US007309594B1

(12) **United States Patent**
Brooun et al.

(10) **Patent No.: US 7,309,594 B1**
(45) **Date of Patent: Dec. 18, 2007**

(54) **CRYSTALLIZATION OF PROTEIN KINASE Bα/AKT1**

(75) Inventors: **Alexei Brooun**, San Diego, CA (US); **Ellen Y. T. Chien**, La Jolla, CA (US); **Douglas R. Dougan**, Calgary (CA); **Andrew J. Jennings**, La Jolla, CA (US); **Michelle L. Kraus**, Temecula, CA (US); **Clifford D. Mol**, San Diego, CA (US)

(73) Assignee: **Takeda San Diego, Inc.**, San Diego, CA (US)

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 360 days.

(21) Appl. No.: **10/842,966**

(22) Filed: **May 10, 2004**

(51) **Int. Cl.**
C12N 9/12 (2006.01)

(52) **U.S. Cl.** **435/194**

(58) **Field of Classification Search** ..... None
See application file for complete search history.

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Primary Examiner—Nashaat T. Nashed
(74) *Attorney, Agent, or Firm*—David J. Weitz

(57) **ABSTRACT**

Provided are crystals relating to Protein kinase Bα/AKT1 and its various uses.

4 Claims, 116 Drawing Sheets

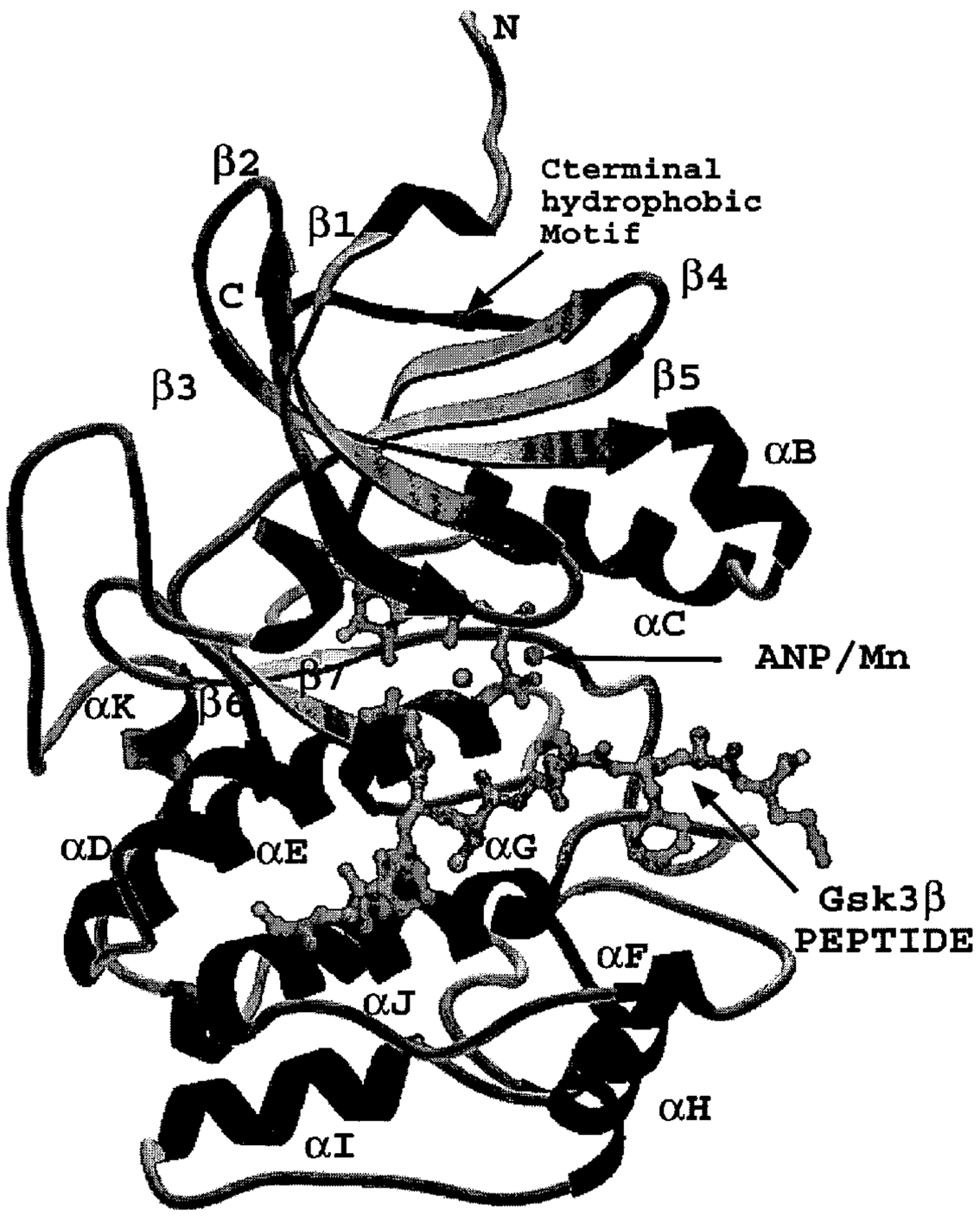

FIGURE 1

Amino acid sequence for full-length human wild type AKT1 [SEQ. ID No. 1]

(Residues 138-480 are underlined)

```
  1 MSDVAIVKEG WLHKRGEYIK TWRPRYFLLK NDGTFIGYKE RPQDVDQREA PLNNFSVAQC
 61 QLMKTERPRP NTFIIRCLQW TTVIERTFHV ETPEEREEWT TAIQTVADGL KKQEEEEMDF
121 RSGSPSDNSG AEEMEVSLAK PKHRVTMNEF EYLKLLGKGT FGKVILVKEK ATGRYYAMKI
181 LKKEVIVAKD EVAHTLTENR VLQNSRHPFL TALKYSFQTH DRLCFVMEYA NGGELFFHLS
241 RERVFSEDRA RFYGAEIVSA LDYLHSEKNV VYRDLKLENL MLDKDGHIKI TDFGLCKEGI
301 KDGATMKTFC GTPEYLAPEV LEDNDYGRAV DWWGLGVVMY EMMCGRLPFY NQDHEKLFEL
361 ILMEEIRFPR TLGPEAKSLL SGLLKKDPKQ RLGGGSEDAK EIMQHRFFAG IVWQHVYEKK
421 LSPPFKPQVT SETDTRYFDE EFTAQMITIT PPDQDDSMEC VDSERRPHFP QFSYSASSTA
```

Human cDNA sequence encoding residues 138-480 of AKT1 [SEQ. ID No. 2]

```
   1 CTGGCCAAGC CCAAGCACCG CGTGACCATG AACGAGTTTG AGTACCTGAA GCTGCTGGGC
  61 AAGGGCACTT TCGGCAAGGT GATCCTGGTG AAGGAGAAGG CCACAGGCCG CTACTACGCC
 121 ATGAAGATCC TCAAGAAGGA AGTCATCGTG GCCAAGGACG AGGTGGCCCA CACACTCACC
 181 GAGAACCGCG TCCTGCAGAA CTCCAGGCAC CCCTTCCTCA CAGCCCTGAA GTACTCTTTC
 241 CAGACCCACG ACCGCCTCTG CTTTGTCATG GAGTACGCCA ACGGGGGCGA GCTGTTCTTC
 301 CACCTGTCCC GGGAACGTGT GTTCTCCGAG GACCGGGCCC GCTTCTATGG CGCTGAGATT
 361 GTGTCAGCCC TGGACTACCT GCACTCGGAG AAGAACGTGG TGTACCGGGA CCTCAAGCTG
 421 GAGAACCTCA TGCTGGACAA GGACGGGCAC ATTAAGATCA CAGACTTCGG GCTGTGCAAG
 481 GAGGGGATCA AGGACGGTGC CACCATGAAG ACCTTTTGCG GCACACCTGA GTACCTGGCC
 541 CCCGAGGTGC TGGAGGACAA TGACTACGGC CGTGCAGTGG ACTGGTGGGG GCTGGGCGTG
 601 GTCATGTACG AGATGATGTG CGGTCGCCTG CCCTTCTACA ACCAGGACCA TGAGAAGCTT
 661 TTTGAGCTCA TCCTCATGGA GGAGATCCGC TTCCCGCGCA CGCTTGGTCC CGAGGCCAAG
 721 TCCTTGCTTT CAGGGCTGCT CAAGAAGGAC CCCAAGCAGA GGCTTGGCGG GGGCTCCGAG
 781 GACGCCAAGG AGATCATGCA GCATCGCTTC TTTGCCGGTA TCGTGTGGCA GCACGTGTAC
 841 GAGAAGAAGC TCAGCCCACC CTTCAAGCCC CAGGTCACGT CGGAGACTGA CACCAGGTAT
 901 TTTGATGAGG AGTTCACGGC CCAGATGATC ACCATCACAC CACCTGACCA AGATGACAGC
 961 ATGGAGTGTG TGGACAGCGA GCGCAGGCCC CACTTCCCCC AGTTCTCCTA CTCGGCCAGC
1021 AGCACGGCCT GA
```

Amino acid sequence for residues 138-480 of AKT1 with a N-terminal 6x-histidine tag, spacer region and rTEV cleavage site [SEQ. ID No. 3]

(6x-histidine tag, spacer region, rTEV cleavage site, M446S, S473D, and (E267-K268-N269) to R267-D268 mutations are underlined)

```
  1 MSYYHHHHHH DYDIPTTENL YFQGAMGSLA KPKHRVTMNE FEYLKLLGKG TFGKVILVKE
 61 KATGRYYAMK ILKKEVIVAK DEVAHTLTEN RVLQNSRHPF LTALKYSFQT HDRLCFVMEY
121 ANGGELFFHL SRERVFSEDR ARFYGAEIVS ALDYLHSRDV VYRDLKLENL MLDKDGHIKI
181 TDFGLCKEGI KDGATMKTFC GTPEYLAPEV LEDNDYGRAV DWWGLGVVMY EMMCGRLPFY
241 NQDHEKLFEL ILMEEIRFPR TLGPEAKSLL SGLLKKDPKQ RLGGGSEDAK EIMQHRFFAG
301 IVWQHVYEKK LSPPFKPQVT SETDTRYFDE EFTAQSITIT PPDQDDSMEC VDSERRPHFP
361 QFDYSASSTA
```

FIGURE 1 (cont.)

Human cDNA sequence encoding SEQ. ID No. 5
[SEQ. ID No. 4]

```
   1 CGCGTGACCA TGAACGAGTT TGAGTACCTG AAGCTGCTGG GCAAGGGCAC TTTCGGCAAG
  61 GTGATCCTGG TGAAGGAGAA GGCCACAGGC CGCTACTACG CCATGAAGAT CCTCAAGAAG
 121 GAAGTCATCG TGGCCAAGGA CGAGGTGGCC CACACACTCA CCGAGAACCG CGTCCTGCAG
 181 AACTCCAGGC ACCCCTTCCT CACAGCCCTG AAGTACTCTT TCCAGACCCA CGACCGCCTC
 241 TGCTTTGTCA TGGAGTACGC CAACGGGGGC GAGCTGTTCT TCCACCTGTC CCGGGAACGT
 301 GTGTTCTCCG AGGACCGGGC CCGCTTCTAT GGCGCTGAGA TTGTGTCAGC CCTGGACTAC
 361 CTGCACTCGG AGAAGAACGT GATGTACCGG GACCTCAAGC TGGAGAACCT CATGCTGGAC
 421 AAGGACGGGC ACATTAAGAT CACAGACTTC GGGCTGTGCA AGGAGGGGAT CAAGGACGGT
 481 GCCACCATGA AGACCTTTTG CGGCACACCT GAGTACCTGG CCCCCGAGGT GCTGGAGGAC
 541 AATGACTACG GCCGTGCAGT GGACTGGTGG GGGCTGGGCG TGGTCATGTA CGAGATGATG
 601 TGCGGTCGCC TGCCCTTCTA CAACCAGGAC CATGAGAAGC TTTTTGAGCT CATCCTCATG
 661 GAGGAGATCC GCTTCCCGCG CACGCTTGGT CCCGAGGCCA AGTCCTTGCT TTCAGGGCTG
 721 CTCAAGAAGG ACCCCAAGCA GAGGCTTGGC GGGGGCTCCG AGGACGCCAA GGAGATCATG
 781 CAGCATCGCT TCTTTGCCGG TATCGTGTGG CAGCACGTGT ACGAGAAGAA GCTCAGCCCA
 841 CCCTTCAAGC CCCAGGTCAC GTCGGAGACT GACACCAGGT ATTTTGATGA GGAGTTCACG
 901 GCCCAGATGA TCACCATCAC ACCACCTGAC CAAGATGACA GCATGGAGTG TGTGGACAGC
 961 GAGCGCGAGG AGCAGGAAAT GTTCAGAGAT TTTGACTACA TTGCTGATTG GTGA
```

Amino acid sequence with a N-terminal 6x-histidine tag, spacer region, rTEV cleavage site, and C-terminal PIFTIDE
[SEQ. ID No. 5]
(6x-histidine tag, spacer region, rTEV cleavage site, and PIFTIDE sequence are underlined)

```
   1 MSYYHHHHHH DYDIPTTENL YFQGAMGSRV TMNEFEYLKL LGKGTFGKVI LVKEKATGRY
  61 YAMKILKKEV IVAKDEVAHT LTENRVLQNS RHPFLTALKY SFQTHDRLCF VMEYANGGEL
 121 FFHLSRERVF SEDRARFYGA EIVSALDYLH SEKNVVYRDL KLENLMLDKD GHIKITDFGL
 181 CKEGIKDGAT MKTFCGTPEY LAPEVLEDND YGRAVDWWGL GVVMYEMMCG RLPFYNQDHE
 241 KLFELILMEE IRFPRTLGPE AKSLLSGLLK KDPKQRLGGG SEDAKEIMQH RFFAGIVWQH
 301 VYEKKLSPPF KPQVTSETDT RYFDEEFTAQ MITITPPDQD DSMECVDSER EEQEMFRDFD
 361 YIADW
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FIGURE 2A

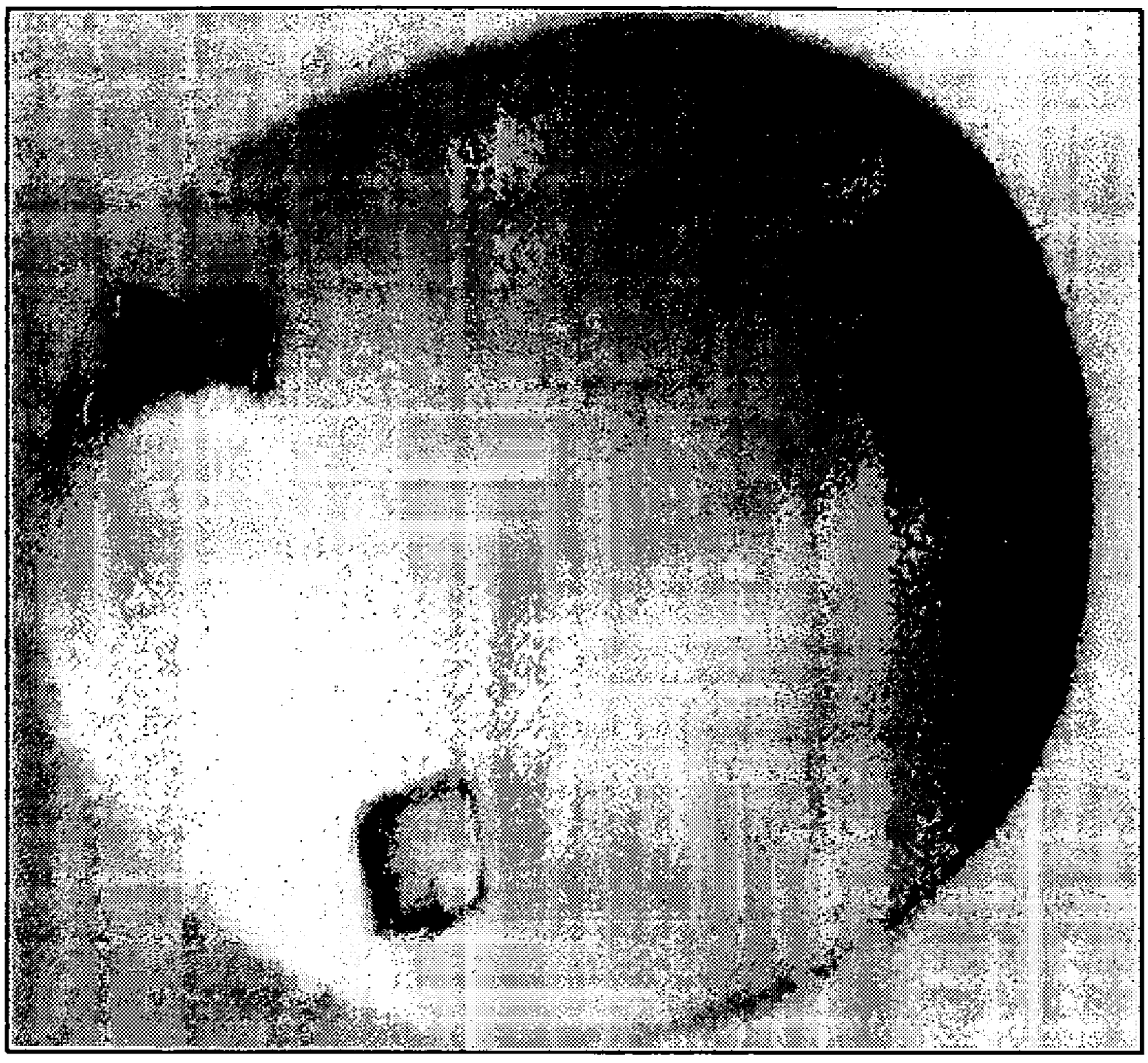


FIGURE 2B

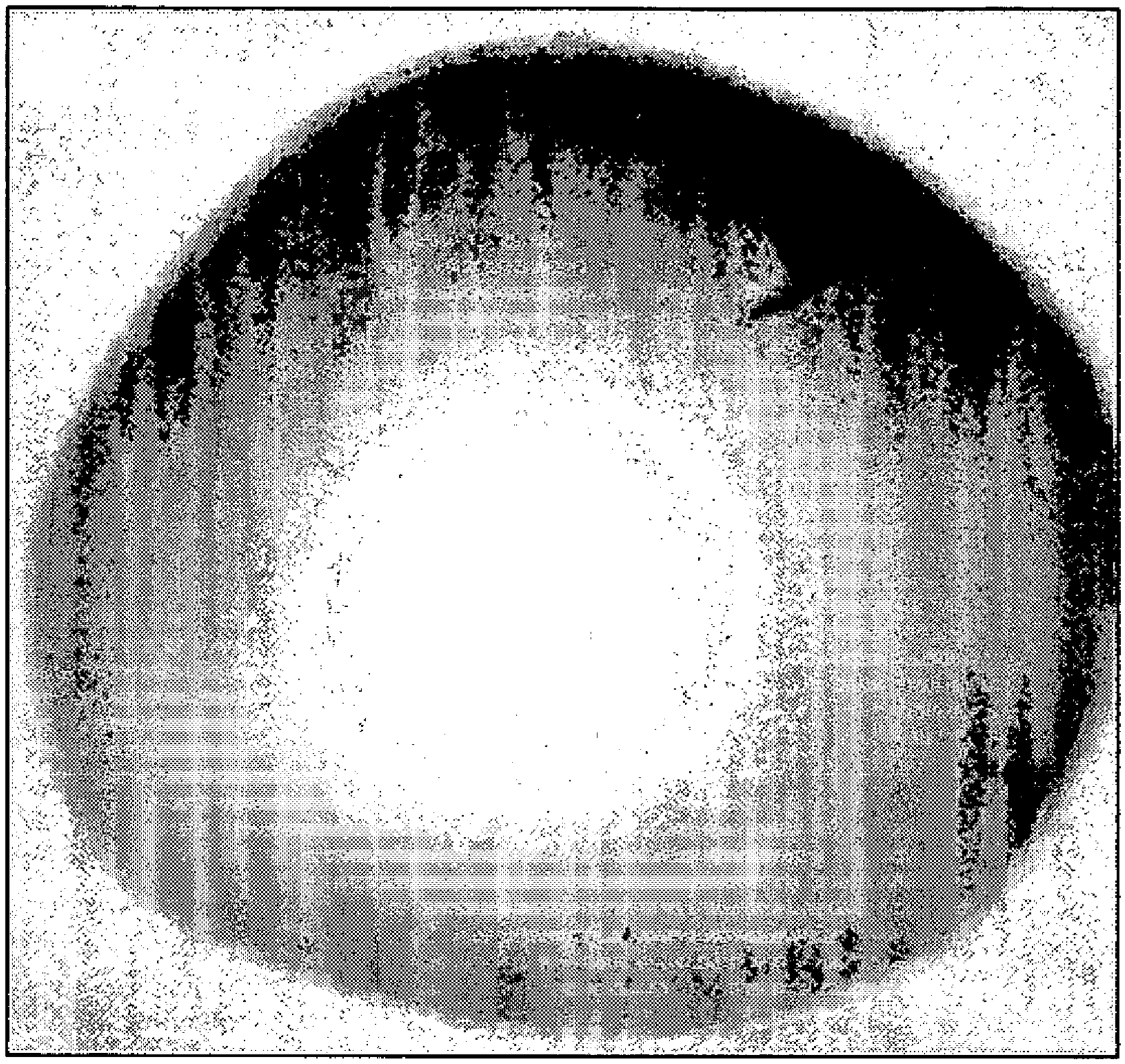


FIGURE 3

LEGEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number', (F)'X Coordinate', (G)'Y Coordinate', (H)'Z Coordinate', (I)'Occupancy' (OCC) and (J)'B factor'.

Molecule A

	A	B	C	D	E	F	G	H	I	J
ATOM	1	N	ALA	A	139	23.707	-17.218	14.088	1.00	86.42
ATOM	2	CA	ALA	A	139	24.409	-15.913	14.293	1.00	87.20
ATOM	3	CB	ALA	A	139	23.636	-14.771	13.614	1.00	84.20
ATOM	4	C	ALA	A	139	24.687	-15.597	15.780	1.00	87.55
ATOM	5	O	ALA	A	139	24.794	-16.509	16.609	1.00	85.62
ATOM	6	N	LYS	A	140	24.785	-14.300	16.094	1.00	89.16
ATOM	7	CA	LYS	A	140	25.305	-13.788	17.374	1.00	89.75
ATOM	8	CB	LYS	A	140	25.347	-12.250	17.318	1.00	88.11
ATOM	9	CG	LYS	A	140	26.307	-11.575	18.308	1.00	89.92
ATOM	10	CD	LYS	A	140	27.748	-11.485	17.785	1.00	89.07
ATOM	11	CE	LYS	A	140	28.207	-10.043	17.570	1.00	89.81
ATOM	12	NZ	LYS	A	140	28.761	-9.428	18.811	1.00	90.51
ATOM	13	C	LYS	A	140	24.527	-14.256	18.617	1.00	91.23
ATOM	14	O	LYS	A	140	23.305	-14.395	18.553	1.00	95.47
ATOM	15	N	PRO	A	141	25.217	-14.515	19.736	1.00	91.45
ATOM	16	CA	PRO	A	141	24.522	-14.767	21.005	1.00	92.04
ATOM	17	CB	PRO	A	141	25.627	-15.313	21.919	1.00	89.78
ATOM	18	CG	PRO	A	141	26.876	-14.718	21.391	1.00	89.68
ATOM	19	CD	PRO	A	141	26.680	-14.601	19.899	1.00	90.79
ATOM	20	C	PRO	A	141	23.947	-13.454	21.549	1.00	93.36
ATOM	21	O	PRO	A	141	24.467	-12.363	21.248	1.00	92.03
ATOM	22	N	LYS	A	142	22.868	-13.566	22.323	1.00	94.37
ATOM	23	CA	LYS	A	142	22.158	-12.384	22.813	1.00	93.56
ATOM	24	CB	LYS	A	142	20.706	-12.696	23.236	1.00	96.03
ATOM	25	CG	LYS	A	142	19.652	-11.709	22.661	1.00	95.69
ATOM	26	CD	LYS	A	142	19.201	-12.082	21.224	1.00	96.14
ATOM	27	CE	LYS	A	142	19.844	-11.197	20.140	1.00	93.86
ATOM	28	NZ	LYS	A	142	19.652	-11.750	18.767	1.00	91.63
ATOM	29	C	LYS	A	142	22.935	-11.686	23.914	1.00	89.37
ATOM	30	O	LYS	A	142	23.560	-12.326	24.766	1.00	87.69
ATOM	31	N	HIS	A	143	22.877	-10.363	23.865	1.00	86.18
ATOM	32	CA	HIS	A	143	23.729	-9.505	24.663	1.00	84.00
ATOM	33	CB	HIS	A	143	23.658	-8.082	24.117	1.00	86.22
ATOM	34	CG	HIS	A	143	24.802	-7.233	24.550	1.00	89.75
ATOM	35	ND1	HIS	A	143	24.643	-6.129	25.359	1.00	90.66
ATOM	36	CE1	HIS	A	143	25.826	-5.588	25.591	1.00	92.24
ATOM	37	NE2	HIS	A	143	26.745	-6.306	24.970	1.00	93.33
ATOM	38	CD2	HIS	A	143	26.131	-7.346	24.316	1.00	91.07
ATOM	39	C	HIS	A	143	23.441	-9.514	26.173	1.00	80.49
ATOM	40	O	HIS	A	143	22.351	-9.139	26.616	1.00	83.46
ATOM	41	N	ARG	A	144	24.430	-9.956	26.948	1.00	72.33

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	42	CA	ARG	A	144	24.422	-9.825	28.402	1.00	63.95
ATOM	43	CB	ARG	A	144	25.702	-10.451	28.977	1.00	65.42
ATOM	44	CG	ARG	A	144	25.639	-10.874	30.443	1.00	66.69
ATOM	45	CD	ARG	A	144	25.071	-12.278	30.680	1.00	67.92
ATOM	46	NE	ARG	A	144	24.818	-12.569	32.098	1.00	68.78
ATOM	47	CZ	ARG	A	144	23.900	-11.965	32.865	1.00	68.79
ATOM	48	NH1	ARG	A	144	23.117	-11.002	32.379	1.00	67.78
ATOM	49	NH2	ARG	A	144	23.771	-12.327	34.136	1.00	68.60
ATOM	50	C	ARG	A	144	24.341	-8.329	28.747	1.00	58.11
ATOM	51	O	ARG	A	144	25.011	-7.508	28.111	1.00	57.25
ATOM	52	N	VAL	A	145	23.508	-7.972	29.725	1.00	51.20
ATOM	53	CA	VAL	A	145	23.340	-6.565	30.112	1.00	43.35
ATOM	54	CB	VAL	A	145	21.856	-6.091	30.054	1.00	39.00
ATOM	55	CG1	VAL	A	145	21.753	-4.628	30.406	1.00	36.52
ATOM	56	CG2	VAL	A	145	21.261	-6.313	28.676	1.00	36.94
ATOM	57	C	VAL	A	145	23.916	-6.302	31.498	1.00	41.85
ATOM	58	O	VAL	A	145	23.728	-7.102	32.423	1.00	40.86
ATOM	59	N	THR	A	146	24.640	-5.190	31.623	1.00	40.26
ATOM	60	CA	THR	A	146	25.147	-4.734	32.919	1.00	39.04
ATOM	61	CB	THR	A	146	26.656	-5.063	33.120	1.00	38.33
ATOM	62	OG1	THR	A	146	27.352	-4.918	31.876	1.00	37.28
ATOM	63	CG2	THR	A	146	26.872	-6.541	33.536	1.00	37.14
ATOM	64	C	THR	A	146	24.930	-3.246	33.121	1.00	36.55
ATOM	65	O	THR	A	146	24.695	-2.497	32.171	1.00	36.01
ATOM	66	N	MET	A	147	25.020	-2.849	34.387	1.00	34.58
ATOM	67	CA	MET	A	147	24.974	-1.468	34.844	1.00	32.48
ATOM	68	CB	MET	A	147	25.687	-1.391	36.199	1.00	34.06
ATOM	69	CG	MET	A	147	24.832	-0.945	37.366	1.00	33.78
ATOM	70	SD	MET	A	147	23.464	-2.046	37.760	1.00	35.32
ATOM	71	CE	MET	A	147	22.424	-0.884	38.683	1.00	32.21
ATOM	72	C	MET	A	147	25.593	-0.436	33.889	1.00	30.63
ATOM	73	O	MET	A	147	25.097	0.684	33.785	1.00	28.59
ATOM	74	N	ASN	A	148	26.667	-0.819	33.198	1.00	30.76
ATOM	75	CA	ASN	A	148	27.484	0.137	32.447	1.00	30.78
ATOM	76	CB	ASN	A	148	28.944	-0.355	32.295	1.00	33.81
ATOM	77	CG	ASN	A	148	29.099	-1.506	31.296	1.00	35.58
ATOM	78	OD1	ASN	A	148	29.451	-1.293	30.131	1.00	36.67
ATOM	79	ND2	ASN	A	148	28.879	-2.731	31.764	1.00	34.81
ATOM	80	C	ASN	A	148	26.907	0.674	31.125	1.00	28.87
ATOM	81	O	ASN	A	148	27.374	1.691	30.621	1.00	28.97
ATOM	82	N	GLU	A	149	25.890	0.004	30.587	1.00	26.92
ATOM	83	CA	GLU	A	149	25.218	0.441	29.358	1.00	27.09
ATOM	84	CB	GLU	A	149	24.420	-0.712	28.778	1.00	30.28
ATOM	85	CG	GLU	A	149	24.960	-1.269	27.489	1.00	34.49
ATOM	86	CD	GLU	A	149	25.156	-2.761	27.598	1.00	38.61
ATOM	87	OE1	GLU	A	149	24.160	-3.468	27.871	1.00	39.64
ATOM	88	OE2	GLU	A	149	26.307	-3.222	27.435	1.00	41.43
ATOM	89	C	GLU	A	149	24.259	1.629	29.542	1.00	25.11
ATOM	90	O	GLU	A	149	23.592	2.047	28.587	1.00	24.91
ATOM	91	N	PHE	A	150	24.179	2.152	30.763	1.00	20.96
ATOM	92	CA	PHE	A	150	23.248	3.222	31.098	1.00	17.83
ATOM	93	CB	PHE	A	150	22.115	2.695	31.980	1.00	15.40

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	94	CG	PHE	A	150	21.375	1.547	31.379	1.00	13.62
ATOM	95	CD1	PHE	A	150	20.236	1.767	30.615	1.00	12.86
ATOM	96	CE1	PHE	A	150	19.550	0.713	30.042	1.00	11.67
ATOM	97	CZ	PHE	A	150	20.007	-0.577	30.225	1.00	13.56
ATOM	98	CE2	PHE	A	150	21.155	-0.811	30.988	1.00	12.96
ATOM	99	CD2	PHE	A	150	21.825	0.246	31.558	1.00	12.00
ATOM	100	C	PHE	A	150	23.958	4.327	31.837	1.00	19.17
ATOM	101	O	PHE	A	150	24.892	4.073	32.591	1.00	20.74
ATOM	102	N	GLU	A	151	23.526	5.559	31.598	1.00	20.45
ATOM	103	CA	GLU	A	151	23.880	6.672	32.466	1.00	19.84
ATOM	104	CB	GLU	A	151	24.109	7.965	31.667	1.00	23.27
ATOM	105	CG	GLU	A	151	25.137	7.837	30.543	1.00	28.78
ATOM	106	CD	GLU	A	151	25.531	9.166	29.893	1.00	32.74
ATOM	107	OE1	GLU	A	151	26.638	9.227	29.290	1.00	33.48
ATOM	108	OE2	GLU	A	151	24.743	10.145	29.966	1.00	33.06
ATOM	109	C	GLU	A	151	22.731	6.803	33.466	1.00	16.14
ATOM	110	O	GLU	A	151	21.612	6.360	33.200	1.00	14.06
ATOM	111	N	TYR	A	152	23.017	7.378	34.625	1.00	13.34
ATOM	112	CA	TYR	A	152	22.022	7.483	35.680	1.00	12.21
ATOM	113	CB	TYR	A	152	22.472	6.684	36.906	1.00	12.73
ATOM	114	CG	TYR	A	152	22.626	5.228	36.580	1.00	13.56
ATOM	115	CD1	TYR	A	152	23.633	4.798	35.722	1.00	16.83
ATOM	116	CE1	TYR	A	152	23.777	3.467	35.382	1.00	16.16
ATOM	117	CZ	TYR	A	152	22.911	2.547	35.892	1.00	15.61
ATOM	118	OH	TYR	A	152	23.085	1.244	35.537	1.00	17.29
ATOM	119	CE2	TYR	A	152	21.887	2.933	36.743	1.00	16.68
ATOM	120	CD2	TYR	A	152	21.750	4.282	37.085	1.00	14.83
ATOM	121	C	TYR	A	152	21.719	8.940	36.003	1.00	12.75
ATOM	122	O	TYR	A	152	22.472	9.605	36.717	1.00	14.73
ATOM	123	N	LEU	A	153	20.597	9.415	35.467	1.00	13.16
ATOM	124	CA	LEU	A	153	20.252	10.834	35.443	1.00	14.90
ATOM	125	CB	LEU	A	153	19.361	11.122	34.236	1.00	19.30
ATOM	126	CG	LEU	A	153	19.996	10.830	32.878	1.00	23.59
ATOM	127	CD1	LEU	A	153	19.039	9.987	32.037	1.00	24.64
ATOM	128	CD2	LEU	A	153	20.400	12.138	32.160	1.00	25.58
ATOM	129	C	LEU	A	153	19.578	11.364	36.707	1.00	12.81
ATOM	130	O	LEU	A	153	20.096	12.291	37.354	1.00	9.78
ATOM	131	N	LYS	A	154	18.414	10.796	37.030	1.00	11.32
ATOM	132	CA	LYS	A	154	17.596	11.258	38.155	1.00	9.86
ATOM	133	CB	LYS	A	154	16.450	12.165	37.673	1.00	9.98
ATOM	134	CG	LYS	A	154	16.867	13.507	37.061	1.00	10.31
ATOM	135	CD	LYS	A	154	16.203	14.680	37.763	1.00	13.90
ATOM	136	CE	LYS	A	154	16.783	16.023	37.298	1.00	18.24
ATOM	137	NZ	LYS	A	154	16.054	17.218	37.853	1.00	19.19
ATOM	138	C	LYS	A	154	17.020	10.092	38.951	1.00	7.31
ATOM	139	O	LYS	A	154	16.674	9.045	38.382	1.00	4.70
ATOM	140	N	LEU	A	155	16.928	10.281	40.268	1.00	5.43
ATOM	141	CA	LEU	A	155	16.225	9.333	41.126	1.00	4.11
ATOM	142	CB	LEU	A	155	16.721	9.384	42.570	1.00	3.10
ATOM	143	CG	LEU	A	155	15.897	8.605	43.606	1.00	3.23
ATOM	144	CD1	LEU	A	155	15.859	7.112	43.294	1.00	5.11
ATOM	145	CD2	LEU	A	155	16.412	8.820	45.021	1.00	2.72

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	146	C	LEU	A	155	14.753	9.665	41.072	1.00	2.79
ATOM	147	O	LEU	A	155	14.353	10.770	41.398	1.00	2.00
ATOM	148	N	LEU	A	156	13.957	8.695	40.642	1.00	5.10
ATOM	149	CA	LEU	A	156	12.538	8.913	40.441	1.00	5.69
ATOM	150	CB	LEU	A	156	12.046	8.149	39.217	1.00	4.03
ATOM	151	CG	LEU	A	156	12.399	8.728	37.853	1.00	2.49
ATOM	152	CD1	LEU	A	156	12.050	7.708	36.797	1.00	2.00
ATOM	153	CD2	LEU	A	156	11.671	10.034	37.604	1.00	2.00
ATOM	154	C	LEU	A	156	11.743	8.481	41.648	1.00	8.44
ATOM	155	O	LEU	A	156	10.686	9.053	41.936	1.00	10.67
ATOM	156	N	GLY	A	157	12.244	7.474	42.355	1.00	9.99
ATOM	157	CA	GLY	A	157	11.471	6.891	43.431	1.00	18.79
ATOM	158	C	GLY	A	157	12.206	5.960	44.360	1.00	23.98
ATOM	159	O	GLY	A	157	13.180	5.315	43.967	1.00	24.19
ATOM	160	N	LYS	A	158	11.724	5.910	45.602	1.00	31.16
ATOM	161	CA	LYS	A	158	12.258	5.030	46.633	1.00	36.62
ATOM	162	CB	LYS	A	158	12.990	5.839	47.709	1.00	37.47
ATOM	163	CG	LYS	A	158	14.465	5.501	47.872	1.00	40.40
ATOM	164	CD	LYS	A	158	14.993	5.976	49.237	1.00	44.44
ATOM	165	CE	LYS	A	158	16.269	6.834	49.122	1.00	45.84
ATOM	166	NZ	LYS	A	158	17.494	6.052	48.729	1.00	44.09
ATOM	167	C	LYS	A	158	11.121	4.212	47.249	1.00	40.37
ATOM	168	O	LYS	A	158	10.151	4.768	47.774	1.00	40.54
ATOM	169	N	GLY	A	159	11.226	2.891	47.110	1.00	44.36
ATOM	170	CA	GLY	A	159	10.483	1.941	47.921	1.00	48.14
ATOM	171	C	GLY	A	159	11.455	1.512	49.011	1.00	52.03
ATOM	172	O	GLY	A	159	12.489	2.170	49.191	1.00	54.97
ATOM	173	N	THR	A	160	11.167	0.428	49.729	1.00	50.92
ATOM	174	CA	THR	A	160	12.011	0.075	50.881	1.00	49.58
ATOM	175	CB	THR	A	160	11.188	-0.639	51.976	1.00	48.94
ATOM	176	OG1	THR	A	160	10.014	0.133	52.258	1.00	49.13
ATOM	177	CG2	THR	A	160	11.929	-0.632	53.309	1.00	48.14
ATOM	178	C	THR	A	160	13.303	-0.694	50.530	1.00	49.71
ATOM	179	O	THR	A	160	14.352	-0.465	51.151	1.00	48.98
ATOM	180	N	PHE	A	161	13.228	-1.585	49.538	1.00	47.64
ATOM	181	CA	PHE	A	161	14.389	-2.385	49.129	1.00	44.58
ATOM	182	CB	PHE	A	161	14.029	-3.874	48.980	1.00	40.85
ATOM	183	CG	PHE	A	161	12.952	-4.340	49.910	1.00	39.69
ATOM	184	CD1	PHE	A	161	11.780	-4.880	49.408	1.00	39.80
ATOM	185	CE1	PHE	A	161	10.766	-5.309	50.263	1.00	40.55
ATOM	186	CZ	PHE	A	161	10.926	-5.199	51.644	1.00	42.20
ATOM	187	CE2	PHE	A	161	12.097	-4.652	52.161	1.00	42.17
ATOM	188	CD2	PHE	A	161	13.106	-4.234	51.294	1.00	41.86
ATOM	189	C	PHE	A	161	14.979	-1.871	47.826	1.00	44.47
ATOM	190	O	PHE	A	161	16.102	-2.247	47.447	1.00	44.46
ATOM	191	N	GLY	A	162	14.227	-0.998	47.155	1.00	43.18
ATOM	192	CA	GLY	A	162	14.510	-0.674	45.770	1.00	42.43
ATOM	193	C	GLY	A	162	14.319	0.748	45.282	1.00	38.55
ATOM	194	O	GLY	A	162	13.238	1.330	45.405	1.00	38.14
ATOM	195	N	LYS	A	163	15.389	1.275	44.690	1.00	33.73
ATOM	196	CA	LYS	A	163	15.383	2.566	44.015	1.00	27.34
ATOM	197	CB	LYS	A	163	16.755	3.221	44.166	1.00	26.23

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	198	CG	LYS	A	163	17.061	3.607	45.588	1.00	29.06
ATOM	199	CD	LYS	A	163	18.023	2.641	46.260	1.00	30.29
ATOM	200	CE	LYS	A	163	18.998	3.400	47.160	1.00	29.25
ATOM	201	NZ	LYS	A	163	20.219	2.604	47.454	1.00	28.10
ATOM	202	C	LYS	A	163	15.003	2.444	42.528	1.00	21.68
ATOM	203	O	LYS	A	163	15.409	1.501	41.840	1.00	19.64
ATOM	204	N	VAL	A	164	14.215	3.401	42.049	1.00	13.68
ATOM	205	CA	VAL	A	164	13.906	3.515	40.638	1.00	9.22
ATOM	206	CB	VAL	A	164	12.426	3.797	40.399	1.00	4.52
ATOM	207	CG1	VAL	A	164	12.154	3.889	38.933	1.00	8.96
ATOM	208	CG2	VAL	A	164	11.582	2.724	40.967	1.00	3.41
ATOM	209	C	VAL	A	164	14.686	4.692	40.086	1.00	13.75
ATOM	210	O	VAL	A	164	14.539	5.822	40.558	1.00	16.43
ATOM	211	N	ILE	A	165	15.510	4.442	39.078	1.00	16.06
ATOM	212	CA	ILE	A	165	16.264	5.528	38.467	1.00	17.85
ATOM	213	CB	ILE	A	165	17.775	5.279	38.594	1.00	19.88
ATOM	214	CG1	ILE	A	165	18.262	5.777	39.956	1.00	22.82
ATOM	215	CD1	ILE	A	165	18.495	4.673	40.984	1.00	25.13
ATOM	216	CG2	ILE	A	165	18.537	5.977	37.482	1.00	18.87
ATOM	217	C	ILE	A	165	15.844	5.752	37.022	1.00	17.16
ATOM	218	O	ILE	A	165	15.517	4.799	36.311	1.00	15.06
ATOM	219	N	LEU	A	166	15.820	7.024	36.618	1.00	16.63
ATOM	220	CA	LEU	A	166	15.517	7.404	35.244	1.00	13.27
ATOM	221	CB	LEU	A	166	14.894	8.794	35.192	1.00	6.52
ATOM	222	CG	LEU	A	166	15.059	9.491	33.852	1.00	4.74
ATOM	223	CD1	LEU	A	166	13.853	9.260	32.971	1.00	4.78
ATOM	224	CD2	LEU	A	166	15.311	10.955	34.068	1.00	4.92
ATOM	225	C	LEU	A	166	16.817	7.378	34.466	1.00	15.72
ATOM	226	O	LEU	A	166	17.671	8.246	34.629	1.00	20.64
ATOM	227	N	VAL	A	167	16.964	6.366	33.627	1.00	16.96
ATOM	228	CA	VAL	A	167	18.216	6.129	32.925	1.00	15.44
ATOM	229	CB	VAL	A	167	18.657	4.630	33.001	1.00	16.81
ATOM	230	CG1	VAL	A	167	18.901	4.192	34.442	1.00	14.89
ATOM	231	CG2	VAL	A	167	17.636	3.713	32.328	1.00	16.18
ATOM	232	C	VAL	A	167	18.113	6.542	31.469	1.00	13.87
ATOM	233	O	VAL	A	167	17.017	6.743	30.933	1.00	13.52
ATOM	234	N	LYS	A	168	19.273	6.680	30.847	1.00	12.62
ATOM	235	CA	LYS	A	168	19.366	6.802	29.411	1.00	13.59
ATOM	236	CB	LYS	A	168	20.009	8.139	29.032	1.00	10.75
ATOM	237	CG	LYS	A	168	19.942	8.493	27.549	1.00	8.86
ATOM	238	CD	LYS	A	168	21.315	8.906	27.006	1.00	10.25
ATOM	239	CE	LYS	A	168	21.631	10.389	27.259	1.00	10.46
ATOM	240	NZ	LYS	A	168	23.061	10.697	26.989	1.00	8.17
ATOM	241	C	LYS	A	168	20.234	5.636	28.974	1.00	15.80
ATOM	242	O	LYS	A	168	21.315	5.437	29.533	1.00	15.67
ATOM	243	N	GLU	A	169	19.749	4.847	28.010	1.00	18.58
ATOM	244	CA	GLU	A	169	20.546	3.763	27.413	1.00	19.15
ATOM	245	CB	GLU	A	169	19.670	2.681	26.769	1.00	19.62
ATOM	246	CG	GLU	A	169	20.341	1.312	26.715	1.00	20.43
ATOM	247	CD	GLU	A	169	19.737	0.368	25.684	1.00	20.48
ATOM	248	OE1	GLU	A	169	18.487	0.342	25.537	1.00	17.12
ATOM	249	OE2	GLU	A	169	20.530	-0.357	25.027	1.00	20.57

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	250	C	GLU	A	169	21.491	4.337	26.380	1.00	18.92
ATOM	251	O	GLU	A	169	21.076	5.086	25.497	1.00	20.97
ATOM	252	N	LYS	A	170	22.762	3.973	26.496	1.00	20.03
ATOM	253	CA	LYS	A	170	23.825	4.573	25.691	1.00	18.18
ATOM	254	CB	LYS	A	170	25.190	4.254	26.303	1.00	17.20
ATOM	255	CG	LYS	A	170	25.527	5.100	27.530	1.00	17.46
ATOM	256	CD	LYS	A	170	26.050	4.233	28.670	1.00	18.36
ATOM	257	CE	LYS	A	170	27.353	4.764	29.245	1.00	20.45
ATOM	258	NZ	LYS	A	170	27.601	4.273	30.628	1.00	20.69
ATOM	259	C	LYS	A	170	23.768	4.169	24.216	1.00	17.61
ATOM	260	O	LYS	A	170	23.883	5.021	23.341	1.00	16.82
ATOM	261	N	ALA	A	171	23.565	2.878	23.954	1.00	19.42
ATOM	262	CA	ALA	A	171	23.522	2.340	22.591	1.00	20.18
ATOM	263	CB	ALA	A	171	23.588	0.795	22.616	1.00	18.65
ATOM	264	C	ALA	A	171	22.343	2.842	21.714	1.00	20.83
ATOM	265	O	ALA	A	171	22.541	3.125	20.524	1.00	21.41
ATOM	266	N	THR	A	172	21.140	2.956	22.288	1.00	20.00
ATOM	267	CA	THR	A	172	19.944	3.341	21.513	1.00	20.37
ATOM	268	CB	THR	A	172	18.711	2.448	21.857	1.00	20.64
ATOM	269	OG1	THR	A	172	18.224	2.758	23.170	1.00	21.43
ATOM	270	CG2	THR	A	172	19.093	0.968	21.948	1.00	20.65
ATOM	271	C	THR	A	172	19.561	4.825	21.618	1.00	21.49
ATOM	272	O	THR	A	172	18.977	5.397	20.686	1.00	21.89
ATOM	273	N	GLY	A	173	19.891	5.439	22.751	1.00	21.37
ATOM	274	CA	GLY	A	173	19.506	6.812	23.029	1.00	20.78
ATOM	275	C	GLY	A	173	18.256	6.852	23.887	1.00	21.56
ATOM	276	O	GLY	A	173	18.083	7.757	24.703	1.00	22.11
ATOM	277	N	ARG	A	174	17.401	5.847	23.703	1.00	21.59
ATOM	278	CA	ARG	A	174	16.112	5.711	24.390	1.00	22.43
ATOM	279	CB	ARG	A	174	15.480	4.364	24.000	1.00	23.24
ATOM	280	CG	ARG	A	174	15.195	4.192	22.490	1.00	24.28
ATOM	281	CD	ARG	A	174	13.704	4.148	22.107	1.00	25.73
ATOM	282	NE	ARG	A	174	12.955	5.251	22.719	1.00	29.66
ATOM	283	CZ	ARG	A	174	12.069	5.115	23.714	1.00	30.98
ATOM	284	NH1	ARG	A	174	11.461	6.188	24.220	1.00	26.56
ATOM	285	NH2	ARG	A	174	11.794	3.907	24.207	1.00	32.07
ATOM	286	C	ARG	A	174	16.151	5.885	25.937	1.00	22.05
ATOM	287	O	ARG	A	174	17.157	5.565	26.581	1.00	21.24
ATOM	288	N	TYR	A	175	15.062	6.407	26.518	1.00	21.57
ATOM	289	CA	TYR	A	175	14.968	6.627	27.976	1.00	19.36
ATOM	290	CB	TYR	A	175	14.478	8.040	28.302	1.00	18.70
ATOM	291	CG	TYR	A	175	15.492	9.115	28.007	1.00	18.35
ATOM	292	CD1	TYR	A	175	15.481	9.794	26.783	1.00	16.50
ATOM	293	CE1	TYR	A	175	16.412	10.774	26.505	1.00	16.96
ATOM	294	CZ	TYR	A	175	17.377	11.093	27.457	1.00	18.83
ATOM	295	OH	TYR	A	175	18.316	12.073	27.186	1.00	21.35
ATOM	296	CE2	TYR	A	175	17.406	10.437	28.681	1.00	17.75
ATOM	297	CD2	TYR	A	175	16.469	9.451	28.947	1.00	17.59
ATOM	298	C	TYR	A	175	14.059	5.625	28.661	1.00	17.75
ATOM	299	O	TYR	A	175	13.036	5.223	28.098	1.00	17.49
ATOM	300	N	TYR	A	176	14.443	5.227	29.874	1.00	15.48
ATOM	301	CA	TYR	A	176	13.700	4.237	30.652	1.00	13.76

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	302	CB	TYR	A	176	14.235	2.819	30.395	1.00	16.36
ATOM	303	CG	TYR	A	176	14.354	2.417	28.932	1.00	17.80
ATOM	304	CD1	TYR	A	176	15.534	2.620	28.231	1.00	16.73
ATOM	305	CE1	TYR	A	176	15.643	2.270	26.906	1.00	18.79
ATOM	306	CZ	TYR	A	176	14.568	1.698	26.259	1.00	20.01
ATOM	307	OH	TYR	A	176	14.682	1.339	24.929	1.00	23.68
ATOM	308	CE2	TYR	A	176	13.389	1.475	26.933	1.00	18.64
ATOM	309	CD2	TYR	A	176	13.286	1.833	28.259	1.00	18.21
ATOM	310	C	TYR	A	176	13.828	4.551	32.131	1.00	12.19
ATOM	311	O	TYR	A	176	14.736	5.273	32.538	1.00	10.58
ATOM	312	N	ALA	A	177	12.908	4.017	32.930	1.00	12.05
ATOM	313	CA	ALA	A	177	13.089	3.970	34.383	1.00	12.59
ATOM	314	CB	ALA	A	177	11.777	4.239	35.100	1.00	9.41
ATOM	315	C	ALA	A	177	13.661	2.599	34.787	1.00	14.88
ATOM	316	O	ALA	A	177	13.148	1.554	34.367	1.00	16.84
ATOM	317	N	MET	A	178	14.733	2.601	35.577	1.00	14.52
ATOM	318	CA	MET	A	178	15.326	1.355	36.057	1.00	13.89
ATOM	319	CB	MET	A	178	16.825	1.325	35.781	1.00	14.22
ATOM	320	CG	MET	A	178	17.438	-0.054	35.890	1.00	16.22
ATOM	321	SD	MET	A	178	19.209	0.012	36.148	1.00	20.29
ATOM	322	CE	MET	A	178	19.790	0.479	34.502	1.00	19.50
ATOM	323	C	MET	A	178	15.058	1.142	37.547	1.00	15.81
ATOM	324	O	MET	A	178	15.402	1.993	38.377	1.00	14.94
ATOM	325	N	LYS	A	179	14.421	0.010	37.867	1.00	16.16
ATOM	326	CA	LYS	A	179	14.197	-0.421	39.245	1.00	12.04
ATOM	327	CB	LYS	A	179	12.907	-1.224	39.379	1.00	7.71
ATOM	328	CG	LYS	A	179	12.197	-0.962	40.684	1.00	5.94
ATOM	329	CD	LYS	A	179	11.652	-2.220	41.295	1.00	6.24
ATOM	330	CE	LYS	A	179	10.145	-2.119	41.529	1.00	8.12
ATOM	331	NZ	LYS	A	179	9.812	-2.080	42.986	1.00	9.56
ATOM	332	C	LYS	A	179	15.364	-1.275	39.667	1.00	12.03
ATOM	333	O	LYS	A	179	15.572	-2.340	39.111	1.00	12.22
ATOM	334	N	ILE	A	180	16.126	-0.786	40.639	1.00	16.15
ATOM	335	CA	ILE	A	180	17.341	-1.446	41.119	1.00	17.67
ATOM	336	CB	ILE	A	180	18.482	-0.408	41.257	1.00	18.26
ATOM	337	CG1	ILE	A	180	19.039	-0.070	39.875	1.00	20.33
ATOM	338	CD1	ILE	A	180	18.931	1.393	39.514	1.00	21.55
ATOM	339	CG2	ILE	A	180	19.603	-0.907	42.165	1.00	17.80
ATOM	340	C	ILE	A	180	17.080	-2.159	42.444	1.00	17.86
ATOM	341	O	ILE	A	180	16.541	-1.567	43.391	1.00	14.98
ATOM	342	N	LEU	A	181	17.468	-3.432	42.505	1.00	16.46
ATOM	343	CA	LEU	A	181	17.287	-4.222	43.720	1.00	14.52
ATOM	344	CB	LEU	A	181	16.239	-5.307	43.485	1.00	14.70
ATOM	345	CG	LEU	A	181	14.834	-4.713	43.324	1.00	17.29
ATOM	346	CD1	LEU	A	181	13.876	-5.653	42.570	1.00	16.60
ATOM	347	CD2	LEU	A	181	14.252	-4.300	44.683	1.00	17.45
ATOM	348	C	LEU	A	181	18.590	-4.816	44.261	1.00	11.71
ATOM	349	O	LEU	A	181	19.366	-5.402	43.526	1.00	10.93
ATOM	350	N	LYS	A	182	18.836	-4.639	45.552	1.00	10.51
ATOM	351	CA	LYS	A	182	19.983	-5.277	46.179	1.00	11.01
ATOM	352	CB	LYS	A	182	20.457	-4.495	47.416	1.00	14.23
ATOM	353	CG	LYS	A	182	20.959	-3.063	47.158	1.00	15.69

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	354	CD	LYS	A	182	22.464	-3.022	46.878	1.00	18.93
ATOM	355	CE	LYS	A	182	23.173	-1.966	47.725	1.00	22.93
ATOM	356	NZ	LYS	A	182	23.710	-0.803	46.938	1.00	23.03
ATOM	357	C	LYS	A	182	19.579	-6.702	46.550	1.00	10.11
ATOM	358	O	LYS	A	182	18.588	-6.905	47.270	1.00	8.75
ATOM	359	N	LYS	A	183	20.322	-7.688	46.037	1.00	8.75
ATOM	360	CA	LYS	A	183	19.984	-9.093	46.275	1.00	4.08
ATOM	361	CB	LYS	A	183	20.852	-10.052	45.469	1.00	2.00
ATOM	362	CG	LYS	A	183	20.735	-9.936	43.985	1.00	2.00
ATOM	363	CD	LYS	A	183	21.924	-10.618	43.345	1.00	2.00
ATOM	364	CE	LYS	A	183	21.627	-11.110	41.940	1.00	2.00
ATOM	365	NZ	LYS	A	183	22.628	-12.117	41.524	1.00	2.00
ATOM	366	C	LYS	A	183	20.162	-9.388	47.737	1.00	3.32
ATOM	367	O	LYS	A	183	19.318	-10.038	48.345	1.00	2.00
ATOM	368	N	GLU	A	184	21.257	-8.886	48.305	1.00	6.85
ATOM	369	CA	GLU	A	184	21.595	-9.167	49.704	1.00	11.76
ATOM	370	CB	GLU	A	184	22.810	-8.347	50.160	1.00	16.12
ATOM	371	CG	GLU	A	184	22.943	-6.983	49.479	1.00	21.94
ATOM	372	CD	GLU	A	184	23.841	-6.020	50.248	1.00	24.70
ATOM	373	OE1	GLU	A	184	24.907	-6.473	50.728	1.00	25.05
ATOM	374	OE2	GLU	A	184	23.490	-4.814	50.371	1.00	24.23
ATOM	375	C	GLU	A	184	20.391	-8.887	50.591	1.00	8.38
ATOM	376	O	GLU	A	184	20.163	-9.576	51.586	1.00	7.73
ATOM	377	N	VAL	A	185	19.620	-7.888	50.167	1.00	4.57
ATOM	378	CA	VAL	A	185	18.472	-7.362	50.886	1.00	2.68
ATOM	379	CB	VAL	A	185	18.236	-5.879	50.515	1.00	2.00
ATOM	380	CG1	VAL	A	185	16.968	-5.335	51.165	1.00	2.00
ATOM	381	CG2	VAL	A	185	19.460	-5.036	50.882	1.00	2.00
ATOM	382	C	VAL	A	185	17.221	-8.174	50.594	1.00	3.44
ATOM	383	O	VAL	A	185	16.513	-8.558	51.523	1.00	4.64
ATOM	384	N	ILE	A	186	16.952	-8.417	49.308	1.00	2.66
ATOM	385	CA	ILE	A	186	15.844	-9.266	48.864	1.00	2.00
ATOM	386	CB	ILE	A	186	15.896	-9.428	47.333	1.00	2.77
ATOM	387	CG1	ILE	A	186	15.614	-8.082	46.643	1.00	7.73
ATOM	388	CD1	ILE	A	186	14.133	-7.577	46.692	1.00	10.02
ATOM	389	CG2	ILE	A	186	14.982	-10.569	46.852	1.00	2.00
ATOM	390	C	ILE	A	186	15.870	-10.638	49.538	1.00	2.00
ATOM	391	O	ILE	A	186	14.838	-11.153	49.967	1.00	2.00
ATOM	392	N	VAL	A	187	17.065	-11.213	49.625	1.00	2.00
ATOM	393	CA	VAL	A	187	17.267	-12.497	50.272	1.00	2.60
ATOM	394	CB	VAL	A	187	18.658	-13.098	49.922	1.00	2.00
ATOM	395	CG1	VAL	A	187	18.892	-14.442	50.624	1.00	2.00
ATOM	396	CG2	VAL	A	187	18.773	-13.278	48.429	1.00	2.00
ATOM	397	C	VAL	A	187	17.045	-12.376	51.785	1.00	5.41
ATOM	398	O	VAL	A	187	16.283	-13.156	52.353	1.00	8.09
ATOM	399	N	ALA	A	188	17.677	-11.388	52.423	1.00	5.56
ATOM	400	CA	ALA	A	188	17.570	-11.217	53.868	1.00	6.01
ATOM	401	CB	ALA	A	188	18.652	-10.290	54.382	1.00	7.78
ATOM	402	C	ALA	A	188	16.189	-10.735	54.304	1.00	8.58
ATOM	403	O	ALA	A	188	15.713	-11.098	55.374	1.00	12.33
ATOM	404	N	LYS	A	189	15.541	-9.928	53.477	1.00	11.57
ATOM	405	CA	LYS	A	189	14.191	-9.466	53.780	1.00	15.35

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	406	CB	LYS	A	189	14.014	-7.995	53.354	1.00	18.39
ATOM	407	CG	LYS	A	189	12.845	-7.255	54.036	1.00	21.90
ATOM	408	CD	LYS	A	189	13.301	-6.228	55.076	1.00	23.27
ATOM	409	CE	LYS	A	189	12.113	-5.688	55.872	1.00	22.64
ATOM	410	NZ	LYS	A	189	11.746	-6.598	57.000	1.00	21.10
ATOM	411	C	LYS	A	189	13.112	-10.382	53.171	1.00	15.74
ATOM	412	O	LYS	A	189	11.922	-10.080	53.233	1.00	18.80
ATOM	413	N	ASP	A	190	13.531	-11.497	52.577	1.00	16.29
ATOM	414	CA	ASP	A	190	12.606	-12.547	52.141	1.00	16.49
ATOM	415	CB	ASP	A	190	11.788	-13.026	53.336	1.00	17.12
ATOM	416	CG	ASP	A	190	11.440	-14.483	53.250	1.00	20.28
ATOM	417	OD1	ASP	A	190	11.449	-15.034	52.125	1.00	22.76
ATOM	418	OD2	ASP	A	190	11.140	-15.157	54.259	1.00	22.17
ATOM	419	C	ASP	A	190	11.664	-12.176	50.988	1.00	15.93
ATOM	420	O	ASP	A	190	10.506	-12.592	50.955	1.00	15.32
ATOM	421	N	GLU	A	191	12.163	-11.406	50.035	1.00	17.29
ATOM	422	CA	GLU	A	191	11.321	-10.935	48.940	1.00	19.49
ATOM	423	CB	GLU	A	191	11.340	-9.407	48.874	1.00	22.95
ATOM	424	CG	GLU	A	191	10.635	-8.724	50.042	1.00	29.33
ATOM	425	CD	GLU	A	191	9.117	-8.619	49.886	1.00	33.52
ATOM	426	OE1	GLU	A	191	8.609	-8.454	48.739	1.00	34.88
ATOM	427	OE2	GLU	A	191	8.427	-8.688	50.934	1.00	34.39
ATOM	428	C	GLU	A	191	11.713	-11.546	47.593	1.00	19.19
ATOM	429	O	GLU	A	191	11.482	-10.958	46.541	1.00	17.18
ATOM	430	N	VAL	A	192	12.312	-12.730	47.633	1.00	20.75
ATOM	431	CA	VAL	A	192	12.689	-13.438	46.418	1.00	17.59
ATOM	432	CB	VAL	A	192	13.599	-14.639	46.743	1.00	14.56
ATOM	433	CG1	VAL	A	192	13.312	-15.828	45.845	1.00	13.35
ATOM	434	CG2	VAL	A	192	15.052	-14.223	46.640	1.00	13.65
ATOM	435	C	VAL	A	192	11.424	-13.846	45.668	1.00	19.48
ATOM	436	O	VAL	A	192	11.221	-13.449	44.517	1.00	18.22
ATOM	437	N	ALA	A	193	10.570	-14.603	46.357	1.00	21.83
ATOM	438	CA	ALA	A	193	9.301	-15.093	45.831	1.00	22.50
ATOM	439	CB	ALA	A	193	8.394	-15.503	46.981	1.00	25.68
ATOM	440	C	ALA	A	193	8.603	-14.059	44.972	1.00	24.14
ATOM	441	O	ALA	A	193	8.143	-14.375	43.866	1.00	26.03
ATOM	442	N	HIS	A	194	8.540	-12.831	45.503	1.00	24.45
ATOM	443	CA	HIS	A	194	7.865	-11.688	44.876	1.00	22.28
ATOM	444	CB	HIS	A	194	7.626	-10.577	45.898	1.00	24.03
ATOM	445	CG	HIS	A	194	6.735	-10.992	47.024	1.00	26.41
ATOM	446	ND1	HIS	A	194	7.211	-11.266	48.287	1.00	26.89
ATOM	447	CE1	HIS	A	194	6.204	-11.621	49.064	1.00	28.79
ATOM	448	NE2	HIS	A	194	5.094	-11.593	48.348	1.00	27.91
ATOM	449	CD2	HIS	A	194	5.400	-11.215	47.065	1.00	26.28
ATOM	450	C	HIS	A	194	8.637	-11.140	43.703	1.00	19.15
ATOM	451	O	HIS	A	194	8.085	-11.033	42.616	1.00	21.49
ATOM	452	N	THR	A	195	9.908	-10.803	43.921	1.00	15.39
ATOM	453	CA	THR	A	195	10.774	-10.353	42.841	1.00	12.03
ATOM	454	CB	THR	A	195	12.255	-10.311	43.243	1.00	10.28
ATOM	455	OG1	THR	A	195	12.420	-9.673	44.507	1.00	10.64
ATOM	456	CG2	THR	A	195	12.987	-9.376	42.326	1.00	12.27
ATOM	457	C	THR	A	195	10.645	-11.256	41.630	1.00	13.09

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	458	O	THR	A	195	10.661	-10.774	40.495	1.00	13.93
ATOM	459	N	LEU	A	196	10.528	-12.565	41.863	1.00	14.82
ATOM	460	CA	LEU	A	196	10.453	-13.524	40.757	1.00	15.21
ATOM	461	CB	LEU	A	196	10.543	-14.961	41.245	1.00	16.66
ATOM	462	CG	LEU	A	196	11.962	-15.511	41.277	1.00	19.79
ATOM	463	CD1	LEU	A	196	11.910	-17.015	41.514	1.00	20.37
ATOM	464	CD2	LEU	A	196	12.729	-15.148	39.985	1.00	21.48
ATOM	465	C	LEU	A	196	9.179	-13.325	39.993	1.00	13.40
ATOM	466	O	LEU	A	196	9.192	-13.236	38.775	1.00	17.14
ATOM	467	N	THR	A	197	8.087	-13.233	40.734	1.00	10.17
ATOM	468	CA	THR	A	197	6.788	-12.957	40.182	1.00	8.59
ATOM	469	CB	THR	A	197	5.828	-12.964	41.324	1.00	9.45
ATOM	470	OG1	THR	A	197	5.492	-14.321	41.605	1.00	15.47
ATOM	471	CG2	THR	A	197	4.518	-12.338	40.927	1.00	14.25
ATOM	472	C	THR	A	197	6.763	-11.614	39.456	1.00	11.50
ATOM	473	O	THR	A	197	6.213	-11.493	38.351	1.00	9.41
ATOM	474	N	GLU	A	198	7.371	-10.608	40.079	1.00	15.61
ATOM	475	CA	GLU	A	198	7.375	-9.257	39.538	1.00	17.76
ATOM	476	CB	GLU	A	198	8.131	-8.309	40.467	1.00	21.98
ATOM	477	CG	GLU	A	198	8.596	-7.030	39.790	1.00	34.80
ATOM	478	CD	GLU	A	198	8.497	-5.798	40.683	1.00	43.72
ATOM	479	OE1	GLU	A	198	8.737	-5.922	41.924	1.00	44.32
ATOM	480	OE2	GLU	A	198	8.188	-4.701	40.125	1.00	46.34
ATOM	481	C	GLU	A	198	7.983	-9.287	38.146	1.00	17.14
ATOM	482	O	GLU	A	198	7.460	-8.672	37.215	1.00	18.91
ATOM	483	N	ASN	A	199	9.076	-10.038	38.025	1.00	14.75
ATOM	484	CA	ASN	A	199	9.786	-10.254	36.775	1.00	11.16
ATOM	485	CB	ASN	A	199	10.997	-11.123	37.089	1.00	13.86
ATOM	486	CG	ASN	A	199	11.863	-11.387	35.892	1.00	18.38
ATOM	487	OD1	ASN	A	199	11.906	-10.592	34.946	1.00	21.95
ATOM	488	ND2	ASN	A	199	12.577	-12.518	35.924	1.00	17.30
ATOM	489	C	ASN	A	199	8.867	-10.944	35.778	1.00	10.73
ATOM	490	O	ASN	A	199	8.544	-10.409	34.717	1.00	7.56
ATOM	491	N	ARG	A	200	8.412	-12.123	36.176	1.00	11.36
ATOM	492	CA	ARG	A	200	7.469	-12.931	35.423	1.00	10.25
ATOM	493	CB	ARG	A	200	6.995	-14.103	36.294	1.00	13.72
ATOM	494	CG	ARG	A	200	7.322	-15.505	35.775	1.00	17.72
ATOM	495	CD	ARG	A	200	6.773	-16.628	36.642	1.00	19.49
ATOM	496	NE	ARG	A	200	7.730	-16.974	37.689	1.00	25.77
ATOM	497	CZ	ARG	A	200	7.531	-16.833	39.002	1.00	28.89
ATOM	498	NH1	ARG	A	200	8.498	-17.190	39.848	1.00	29.58
ATOM	499	NH2	ARG	A	200	6.386	-16.345	39.478	1.00	27.11
ATOM	500	C	ARG	A	200	6.267	-12.149	34.891	1.00	8.77
ATOM	501	O	ARG	A	200	5.854	-12.381	33.760	1.00	11.18
ATOM	502	N	VAL	A	201	5.689	-11.243	35.681	1.00	6.46
ATOM	503	CA	VAL	A	201	4.491	-10.550	35.198	1.00	9.17
ATOM	504	CB	VAL	A	201	3.672	-9.845	36.308	1.00	8.28
ATOM	505	CG1	VAL	A	201	2.684	-8.879	35.697	1.00	3.97
ATOM	506	CG2	VAL	A	201	2.919	-10.853	37.148	1.00	11.11
ATOM	507	C	VAL	A	201	4.906	-9.548	34.145	1.00	10.71
ATOM	508	O	VAL	A	201	4.547	-9.681	32.980	1.00	10.91
ATOM	509	N	LEU	A	202	5.686	-8.562	34.577	1.00	12.99

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	510	CA	LEU	A	202	6.220	-7.517	33.720	1.00	13.14
ATOM	511	CB	LEU	A	202	7.449	-6.921	34.375	1.00	7.21
ATOM	512	CG	LEU	A	202	7.267	-5.795	35.347	1.00	3.69
ATOM	513	CD1	LEU	A	202	8.537	-5.705	36.170	1.00	5.33
ATOM	514	CD2	LEU	A	202	7.034	-4.524	34.579	1.00	3.90
ATOM	515	C	LEU	A	202	6.658	-8.080	32.380	1.00	15.64
ATOM	516	O	LEU	A	202	6.608	-7.400	31.348	1.00	18.52
ATOM	517	N	GLN	A	203	7.112	-9.325	32.422	1.00	12.64
ATOM	518	CA	GLN	A	203	7.701	-9.952	31.274	1.00	13.55
ATOM	519	CB	GLN	A	203	8.468	-11.178	31.725	1.00	11.38
ATOM	520	CG	GLN	A	203	9.929	-11.095	31.488	1.00	7.78
ATOM	521	CD	GLN	A	203	10.594	-12.400	31.741	1.00	6.69
ATOM	522	OE1	GLN	A	203	10.422	-13.363	30.979	1.00	4.01
ATOM	523	NE2	GLN	A	203	11.354	-12.458	32.824	1.00	8.36
ATOM	524	C	GLN	A	203	6.612	-10.381	30.328	1.00	18.36
ATOM	525	O	GLN	A	203	6.735	-10.221	29.113	1.00	22.07
ATOM	526	N	ASN	A	204	5.539	-10.916	30.898	1.00	21.83
ATOM	527	CA	ASN	A	204	4.512	-11.606	30.130	1.00	25.11
ATOM	528	CB	ASN	A	204	4.070	-12.855	30.892	1.00	24.51
ATOM	529	CG	ASN	A	204	4.946	-14.049	30.605	1.00	24.50
ATOM	530	OD1	ASN	A	204	4.542	-15.186	30.843	1.00	28.55
ATOM	531	ND2	ASN	A	204	6.154	-13.804	30.094	1.00	20.02
ATOM	532	C	ASN	A	204	3.292	-10.751	29.786	1.00	27.01
ATOM	533	O	ASN	A	204	2.403	-11.187	29.048	1.00	28.04
ATOM	534	N	SER	A	205	3.259	-9.536	30.318	1.00	26.56
ATOM	535	CA	SER	A	205	2.043	-8.755	30.310	1.00	25.06
ATOM	536	CB	SER	A	205	1.784	-8.209	31.705	1.00	24.45
ATOM	537	OG	SER	A	205	1.453	-9.274	32.576	1.00	23.55
ATOM	538	C	SER	A	205	2.111	-7.649	29.280	1.00	27.77
ATOM	539	O	SER	A	205	2.896	-6.701	29.411	1.00	35.42
ATOM	540	N	ARG	A	206	1.267	-7.783	28.260	1.00	23.70
ATOM	541	CA	ARG	A	206	1.234	-6.882	27.121	1.00	19.49
ATOM	542	CB	ARG	A	206	1.427	-7.715	25.834	1.00	22.78
ATOM	543	CG	ARG	A	206	2.775	-7.544	25.064	1.00	27.32
ATOM	544	CD	ARG	A	206	4.066	-7.895	25.834	1.00	27.84
ATOM	545	NE	ARG	A	206	4.742	-9.090	25.315	1.00	29.21
ATOM	546	CZ	ARG	A	206	5.945	-9.516	25.712	1.00	29.95
ATOM	547	NH1	ARG	A	206	6.636	-8.845	26.622	1.00	31.56
ATOM	548	NH2	ARG	A	206	6.467	-10.622	25.203	1.00	29.69
ATOM	549	C	ARG	A	206	-0.106	-6.117	27.113	1.00	13.59
ATOM	550	O	ARG	A	206	-1.107	-6.619	26.623	1.00	17.68
ATOM	551	N	HIS	A	207	-0.130	-4.908	27.661	1.00	5.11
ATOM	552	CA	HIS	A	207	-1.379	-4.146	27.772	1.00	4.65
ATOM	553	CB	HIS	A	207	-2.109	-4.513	29.061	1.00	3.92
ATOM	554	CG	HIS	A	207	-3.456	-3.877	29.201	1.00	2.57
ATOM	555	ND1	HIS	A	207	-4.626	-4.541	28.900	1.00	4.52
ATOM	556	CE1	HIS	A	207	-5.655	-3.742	29.119	1.00	3.68
ATOM	557	NE2	HIS	A	207	-5.193	-2.581	29.546	1.00	3.88
ATOM	558	CD2	HIS	A	207	-3.821	-2.642	29.610	1.00	2.70
ATOM	559	C	HIS	A	207	-1.108	-2.646	27.752	1.00	7.08
ATOM	560	O	HIS	A	207	-0.122	-2.201	28.314	1.00	14.05
ATOM	561	N	PRO	A	208	-1.966	-1.851	27.118	1.00	8.27

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	562	CA	PRO	A	208	-1.694	-0.420	26.977	1.00	9.24
ATOM	563	CB	PRO	A	208	-2.946	0.086	26.269	1.00	8.40
ATOM	564	CG	PRO	A	208	-3.974	-0.939	26.571	1.00	6.67
ATOM	565	CD	PRO	A	208	-3.238	-2.216	26.469	1.00	8.30
ATOM	566	C	PRO	A	208	-1.495	0.309	28.316	1.00	12.90
ATOM	567	O	PRO	A	208	-0.768	1.306	28.345	1.00	14.64
ATOM	568	N	PHE	A	209	-2.108	-0.192	29.390	1.00	12.89
ATOM	569	CA	PHE	A	209	-2.090	0.473	30.692	1.00	10.18
ATOM	570	CB	PHE	A	209	-3.515	0.684	31.177	1.00	4.84
ATOM	571	CG	PHE	A	209	-4.400	1.267	30.152	1.00	5.70
ATOM	572	CD1	PHE	A	209	-4.028	2.434	29.486	1.00	7.79
ATOM	573	CE1	PHE	A	209	-4.853	2.995	28.517	1.00	8.32
ATOM	574	CZ	PHE	A	209	-6.076	2.372	28.204	1.00	9.16
ATOM	575	CE2	PHE	A	209	-6.452	1.196	28.864	1.00	7.28
ATOM	576	CD2	PHE	A	209	-5.606	0.652	29.828	1.00	7.12
ATOM	577	C	PHE	A	209	-1.284	-0.280	31.748	1.00	13.63
ATOM	578	O	PHE	A	209	-1.406	-0.030	32.958	1.00	19.21
ATOM	579	N	LEU	A	210	-0.467	-1.217	31.303	1.00	9.08
ATOM	580	CA	LEU	A	210	0.481	-1.804	32.214	1.00	11.05
ATOM	581	CB	LEU	A	210	0.346	-3.320	32.219	1.00	11.28
ATOM	582	CG	LEU	A	210	-0.949	-3.904	32.793	1.00	12.46
ATOM	583	CD1	LEU	A	210	-0.794	-5.401	33.002	1.00	10.13
ATOM	584	CD2	LEU	A	210	-1.412	-3.201	34.087	1.00	10.62
ATOM	585	C	LEU	A	210	1.871	-1.367	31.793	1.00	15.31
ATOM	586	O	LEU	A	210	2.135	-1.215	30.596	1.00	18.78
ATOM	587	N	THR	A	211	2.755	-1.147	32.766	1.00	15.52
ATOM	588	CA	THR	A	211	4.130	-0.768	32.462	1.00	17.90
ATOM	589	CB	THR	A	211	4.885	-0.375	33.727	1.00	21.77
ATOM	590	OG1	THR	A	211	3.995	0.317	34.605	1.00	26.09
ATOM	591	CG2	THR	A	211	5.913	0.702	33.417	1.00	26.87
ATOM	592	C	THR	A	211	4.843	-1.892	31.725	1.00	17.49
ATOM	593	O	THR	A	211	4.799	-3.048	32.152	1.00	18.80
ATOM	594	N	ALA	A	212	5.462	-1.539	30.598	1.00	15.19
ATOM	595	CA	ALA	A	212	6.134	-2.490	29.719	1.00	12.51
ATOM	596	CB	ALA	A	212	6.055	-2.012	28.286	1.00	10.74
ATOM	597	C	ALA	A	212	7.585	-2.681	30.133	1.00	12.36
ATOM	598	O	ALA	A	212	8.287	-1.709	30.414	1.00	9.72
ATOM	599	N	LEU	A	213	8.030	-3.934	30.177	1.00	14.72
ATOM	600	CA	LEU	A	213	9.420	-4.225	30.529	1.00	17.99
ATOM	601	CB	LEU	A	213	9.529	-5.479	31.413	1.00	17.23
ATOM	602	CG	LEU	A	213	10.927	-6.037	31.714	1.00	15.27
ATOM	603	CD1	LEU	A	213	11.623	-5.229	32.780	1.00	16.34
ATOM	604	CD2	LEU	A	213	10.823	-7.481	32.153	1.00	15.33
ATOM	605	C	LEU	A	213	10.276	-4.358	29.276	1.00	20.60
ATOM	606	O	LEU	A	213	9.894	-5.064	28.320	1.00	19.97
ATOM	607	N	LYS	A	214	11.418	-3.658	29.294	1.00	22.83
ATOM	608	CA	LYS	A	214	12.379	-3.630	28.180	1.00	23.96
ATOM	609	CB	LYS	A	214	12.905	-2.207	27.940	1.00	22.99
ATOM	610	CG	LYS	A	214	14.133	-2.124	27.033	1.00	25.04
ATOM	611	CD	LYS	A	214	13.750	-2.032	25.539	1.00	26.92
ATOM	612	CE	LYS	A	214	14.865	-2.523	24.612	1.00	23.84
ATOM	613	NZ	LYS	A	214	14.378	-3.518	23.612	1.00	23.78

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	614	C	LYS	A	214	13.542	-4.585	28.433	1.00	24.84
ATOM	615	O	LYS	A	214	13.805	-5.481	27.622	1.00	25.03
ATOM	616	N	TYR	A	215	14.239	-4.369	29.549	1.00	23.99
ATOM	617	CA	TYR	A	215	15.278	-5.276	30.018	1.00	21.25
ATOM	618	CB	TYR	A	215	16.672	-4.652	29.911	1.00	19.04
ATOM	619	CG	TYR	A	215	17.087	-4.151	28.557	1.00	18.19
ATOM	620	CD1	TYR	A	215	17.022	-4.966	27.434	1.00	18.49
ATOM	621	CE1	TYR	A	215	17.418	-4.497	26.184	1.00	19.88
ATOM	622	CZ	TYR	A	215	17.899	-3.203	26.060	1.00	20.21
ATOM	623	OH	TYR	A	215	18.293	-2.729	24.830	1.00	22.62
ATOM	624	CE2	TYR	A	215	17.988	-2.383	27.166	1.00	20.01
ATOM	625	CD2	TYR	A	215	17.586	-2.862	28.408	1.00	18.95
ATOM	626	C	TYR	A	215	15.055	-5.613	31.481	1.00	21.19
ATOM	627	O	TYR	A	215	14.675	-4.752	32.280	1.00	20.20
ATOM	628	N	SER	A	216	15.310	-6.869	31.823	1.00	18.31
ATOM	629	CA	SER	A	216	15.540	-7.242	33.200	1.00	16.18
ATOM	630	CB	SER	A	216	14.377	-8.055	33.739	1.00	16.79
ATOM	631	OG	SER	A	216	14.590	-9.434	33.548	1.00	18.82
ATOM	632	C	SER	A	216	16.837	-8.032	33.232	1.00	17.13
ATOM	633	O	SER	A	216	16.990	-8.993	32.496	1.00	17.99
ATOM	634	N	PHE	A	217	17.782	-7.603	34.064	1.00	19.20
ATOM	635	CA	PHE	A	217	19.101	-8.240	34.144	1.00	16.30
ATOM	636	CB	PHE	A	217	20.106	-7.498	33.262	1.00	12.42
ATOM	637	CG	PHE	A	217	20.371	-6.083	33.699	1.00	11.83
ATOM	638	CD1	PHE	A	217	19.562	-5.042	33.261	1.00	11.69
ATOM	639	CE1	PHE	A	217	19.808	-3.725	33.658	1.00	11.93
ATOM	640	CZ	PHE	A	217	20.876	-3.441	34.504	1.00	12.79
ATOM	641	CE2	PHE	A	217	21.695	-4.474	34.951	1.00	12.87
ATOM	642	CD2	PHE	A	217	21.440	-5.788	34.543	1.00	12.76
ATOM	643	C	PHE	A	217	19.598	-8.313	35.594	1.00	16.91
ATOM	644	O	PHE	A	217	18.994	-7.690	36.497	1.00	17.16
ATOM	645	N	GLN	A	218	20.674	-9.079	35.817	1.00	10.91
ATOM	646	CA	GLN	A	218	21.285	-9.165	37.146	1.00	6.42
ATOM	647	CB	GLN	A	218	20.864	-10.433	37.899	1.00	4.74
ATOM	648	CG	GLN	A	218	21.708	-11.683	37.621	1.00	3.09
ATOM	649	CD	GLN	A	218	21.054	-12.964	38.116	1.00	2.00
ATOM	650	OE1	GLN	A	218	21.044	-13.246	39.312	1.00	2.00
ATOM	651	NE2	GLN	A	218	20.506	-13.733	37.200	1.00	2.00
ATOM	652	C	GLN	A	218	22.794	-9.047	37.097	1.00	7.78
ATOM	653	O	GLN	A	218	23.440	-9.568	36.185	1.00	7.07
ATOM	654	N	THR	A	219	23.327	-8.329	38.085	1.00	10.09
ATOM	655	CA	THR	A	219	24.760	-8.150	38.293	1.00	12.25
ATOM	656	CB	THR	A	219	25.076	-6.691	38.709	1.00	13.22
ATOM	657	OG1	THR	A	219	24.258	-6.322	39.824	1.00	13.71
ATOM	658	CG2	THR	A	219	24.667	-5.701	37.635	1.00	14.64
ATOM	659	C	THR	A	219	25.176	-9.103	39.409	1.00	12.92
ATOM	660	O	THR	A	219	24.410	-10.002	39.765	1.00	11.32
ATOM	661	N	HIS	A	220	26.376	-8.914	39.960	1.00	14.53
ATOM	662	CA	HIS	A	220	26.773	-9.654	41.159	1.00	18.28
ATOM	663	CB	HIS	A	220	28.267	-9.468	41.522	1.00	24.00
ATOM	664	CG	HIS	A	220	28.893	-8.199	41.005	1.00	31.28
ATOM	665	ND1	HIS	A	220	30.108	-8.184	40.348	1.00	35.42

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	666	CE1	HIS	A	220	30.424	-6.940	40.028	1.00	34.54
ATOM	667	NE2	HIS	A	220	29.464	-6.143	40.463	1.00	33.64
ATOM	668	CD2	HIS	A	220	28.500	-6.903	41.086	1.00	32.64
ATOM	669	C	HIS	A	220	25.857	-9.355	42.366	1.00	16.57
ATOM	670	O	HIS	A	220	25.497	-10.263	43.121	1.00	14.27
ATOM	671	N	ASP	A	221	25.457	-8.092	42.514	1.00	15.94
ATOM	672	CA	ASP	A	221	24.796	-7.620	43.732	1.00	16.25
ATOM	673	CB	ASP	A	221	25.626	-6.527	44.431	1.00	22.55
ATOM	674	CG	ASP	A	221	26.212	-5.498	43.461	1.00	28.05
ATOM	675	OD1	ASP	A	221	25.601	-5.230	42.395	1.00	30.06
ATOM	676	OD2	ASP	A	221	27.290	-4.899	43.697	1.00	29.84
ATOM	677	C	ASP	A	221	23.388	-7.108	43.522	1.00	13.08
ATOM	678	O	ASP	A	221	22.632	-6.955	44.483	1.00	12.33
ATOM	679	N	ARG	A	222	23.036	-6.840	42.272	1.00	10.45
ATOM	680	CA	ARG	A	222	21.752	-6.219	41.991	1.00	10.85
ATOM	681	CB	ARG	A	222	21.940	-4.794	41.443	1.00	13.32
ATOM	682	CG	ARG	A	222	22.544	-3.772	42.417	1.00	12.17
ATOM	683	CD	ARG	A	222	23.394	-2.739	41.708	1.00	12.56
ATOM	684	NE	ARG	A	222	24.347	-2.060	42.578	1.00	13.85
ATOM	685	CZ	ARG	A	222	24.225	-0.797	42.974	1.00	15.21
ATOM	686	NH1	ARG	A	222	23.176	-0.072	42.600	1.00	16.45
ATOM	687	NH2	ARG	A	222	25.146	-0.256	43.755	1.00	15.42
ATOM	688	C	ARG	A	222	20.878	-7.015	41.037	1.00	9.25
ATOM	689	O	ARG	A	222	21.371	-7.707	40.150	1.00	11.73
ATOM	690	N	LEU	A	223	19.571	-6.920	41.255	1.00	7.95
ATOM	691	CA	LEU	A	223	18.582	-7.266	40.250	1.00	5.79
ATOM	692	CB	LEU	A	223	17.430	-8.055	40.845	1.00	2.99
ATOM	693	CG	LEU	A	223	17.876	-9.270	41.625	1.00	2.31
ATOM	694	CD1	LEU	A	223	16.745	-9.689	42.514	1.00	5.68
ATOM	695	CD2	LEU	A	223	18.288	-10.382	40.691	1.00	2.00
ATOM	696	C	LEU	A	223	18.067	-5.966	39.693	1.00	6.90
ATOM	697	O	LEU	A	223	17.958	-4.972	40.423	1.00	3.04
ATOM	698	N	CYS	A	224	17.754	-5.984	38.398	1.00	10.76
ATOM	699	CA	CYS	A	224	17.418	-4.771	37.675	1.00	13.46
ATOM	700	CB	CYS	A	224	18.636	-4.265	36.934	1.00	15.09
ATOM	701	SG	CYS	A	224	19.705	-3.287	37.982	1.00	23.17
ATOM	702	C	CYS	A	224	16.303	-4.940	36.683	1.00	13.74
ATOM	703	O	CYS	A	224	16.427	-5.721	35.742	1.00	16.00
ATOM	704	N	PHE	A	225	15.222	-4.195	36.891	1.00	12.21
ATOM	705	CA	PHE	A	225	14.208	-4.033	35.868	1.00	11.81
ATOM	706	CB	PHE	A	225	12.826	-4.147	36.459	1.00	14.09
ATOM	707	CG	PHE	A	225	12.565	-5.423	37.169	1.00	14.19
ATOM	708	CD1	PHE	A	225	12.423	-5.440	38.548	1.00	14.88
ATOM	709	CE1	PHE	A	225	12.144	-6.615	39.230	1.00	13.51
ATOM	710	CZ	PHE	A	225	11.986	-7.782	38.532	1.00	14.88
ATOM	711	CE2	PHE	A	225	12.113	-7.778	37.140	1.00	16.65
ATOM	712	CD2	PHE	A	225	12.392	-6.593	36.467	1.00	15.37
ATOM	713	C	PHE	A	225	14.326	-2.663	35.186	1.00	12.12
ATOM	714	O	PHE	A	225	14.347	-1.615	35.847	1.00	5.03
ATOM	715	N	VAL	A	226	14.402	-2.697	33.854	1.00	12.07
ATOM	716	CA	VAL	A	226	14.371	-1.506	33.020	1.00	8.03
ATOM	717	CB	VAL	A	226	15.458	-1.549	31.972	1.00	5.66

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	718	CG1	VAL	A	226	15.666	-0.168	31.393	1.00	5.17
ATOM	719	CG2	VAL	A	226	16.743	-2.103	32.562	1.00	5.62
ATOM	720	C	VAL	A	226	13.033	-1.458	32.312	1.00	9.28
ATOM	721	O	VAL	A	226	12.806	-2.173	31.337	1.00	8.28
ATOM	722	N	MET	A	227	12.135	-0.634	32.825	1.00	12.05
ATOM	723	CA	MET	A	227	10.811	-0.525	32.244	1.00	16.06
ATOM	724	CB	MET	A	227	9.721	-0.903	33.249	1.00	21.27
ATOM	725	CG	MET	A	227	9.591	0.001	34.446	1.00	24.93
ATOM	726	SD	MET	A	227	9.527	-1.061	35.855	1.00	31.99
ATOM	727	CE	MET	A	227	9.029	0.085	37.161	1.00	29.11
ATOM	728	C	MET	A	227	10.571	0.853	31.667	1.00	15.33
ATOM	729	O	MET	A	227	11.422	1.747	31.790	1.00	13.47
ATOM	730	N	GLU	A	228	9.414	1.017	31.030	1.00	14.08
ATOM	731	CA	GLU	A	228	9.165	2.225	30.282	1.00	15.90
ATOM	732	CB	GLU	A	228	8.082	2.025	29.218	1.00	22.01
ATOM	733	CG	GLU	A	228	6.649	2.246	29.686	1.00	34.10
ATOM	734	CD	GLU	A	228	5.629	1.562	28.785	1.00	41.38
ATOM	735	OE1	GLU	A	228	5.738	1.713	27.546	1.00	42.83
ATOM	736	OE2	GLU	A	228	4.719	0.864	29.310	1.00	44.92
ATOM	737	C	GLU	A	228	8.828	3.307	31.263	1.00	12.11
ATOM	738	O	GLU	A	228	7.907	3.158	32.047	1.00	13.79
ATOM	739	N	TYR	A	229	9.626	4.371	31.227	1.00	11.73
ATOM	740	CA	TYR	A	229	9.421	5.603	31.994	1.00	13.35
ATOM	741	CB	TYR	A	229	10.469	6.610	31.541	1.00	13.11
ATOM	742	CG	TYR	A	229	10.439	7.970	32.209	1.00	13.35
ATOM	743	CD1	TYR	A	229	10.270	8.111	33.587	1.00	12.43
ATOM	744	CE1	TYR	A	229	10.266	9.373	34.180	1.00	12.97
ATOM	745	CZ	TYR	A	229	10.449	10.502	33.392	1.00	12.63
ATOM	746	OH	TYR	A	229	10.462	11.759	33.939	1.00	12.80
ATOM	747	CE2	TYR	A	229	10.619	10.382	32.038	1.00	13.97
ATOM	748	CD2	TYR	A	229	10.621	9.122	31.453	1.00	14.34
ATOM	749	C	TYR	A	229	8.040	6.241	31.825	1.00	13.03
ATOM	750	O	TYR	A	229	7.563	6.434	30.711	1.00	15.41
ATOM	751	N	ALA	A	230	7.409	6.604	32.927	1.00	11.02
ATOM	752	CA	ALA	A	230	6.122	7.273	32.836	1.00	14.49
ATOM	753	CB	ALA	A	230	5.132	6.562	33.707	1.00	14.72
ATOM	754	C	ALA	A	230	6.197	8.786	33.175	1.00	18.02
ATOM	755	O	ALA	A	230	5.917	9.197	34.306	1.00	22.60
ATOM	756	N	ASN	A	231	6.566	9.594	32.178	1.00	16.28
ATOM	757	CA	ASN	A	231	6.748	11.042	32.298	1.00	15.09
ATOM	758	CB	ASN	A	231	6.626	11.692	30.917	1.00	22.58
ATOM	759	CG	ASN	A	231	7.770	11.328	29.980	1.00	29.16
ATOM	760	OD1	ASN	A	231	8.741	12.089	29.832	1.00	31.83
ATOM	761	ND2	ASN	A	231	7.648	10.175	29.315	1.00	30.67
ATOM	762	C	ASN	A	231	5.806	11.792	33.249	1.00	15.62
ATOM	763	O	ASN	A	231	6.221	12.776	33.889	1.00	16.15
ATOM	764	N	GLY	A	232	4.550	11.342	33.328	1.00	13.50
ATOM	765	CA	GLY	A	232	3.486	12.078	34.001	1.00	13.31
ATOM	766	C	GLY	A	232	3.313	11.864	35.497	1.00	15.07
ATOM	767	O	GLY	A	232	2.338	12.348	36.087	1.00	16.07
ATOM	768	N	GLY	A	233	4.240	11.133	36.112	1.00	12.98
ATOM	769	CA	GLY	A	233	4.255	10.975	37.554	1.00	14.96

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	770	C	GLY	A	233	3.155	10.090	38.089	1.00	16.36
ATOM	771	O	GLY	A	233	2.380	9.532	37.315	1.00	17.11
ATOM	772	N	GLU	A	234	3.095	9.945	39.413	1.00	16.83
ATOM	773	CA	GLU	A	234	2.067	9.111	40.031	1.00	14.46
ATOM	774	CB	GLU	A	234	2.517	8.542	41.364	1.00	15.78
ATOM	775	CG	GLU	A	234	4.009	8.550	41.626	1.00	19.92
ATOM	776	CD	GLU	A	234	4.294	8.254	43.088	1.00	22.18
ATOM	777	OE1	GLU	A	234	4.054	9.154	43.923	1.00	25.14
ATOM	778	OE2	GLU	A	234	4.730	7.125	43.412	1.00	20.01
ATOM	779	C	GLU	A	234	0.783	9.888	40.241	1.00	12.81
ATOM	780	O	GLU	A	234	0.801	11.115	40.343	1.00	12.19
ATOM	781	N	LEU	A	235	-0.336	9.174	40.304	1.00	10.87
ATOM	782	CA	LEU	A	235	-1.612	9.834	40.515	1.00	8.65
ATOM	783	CB	LEU	A	235	-2.779	8.853	40.438	1.00	4.06
ATOM	784	CG	LEU	A	235	-3.327	8.660	39.022	1.00	2.00
ATOM	785	CD1	LEU	A	235	-4.546	7.765	39.018	1.00	2.00
ATOM	786	CD2	LEU	A	235	-3.660	9.994	38.368	1.00	2.00
ATOM	787	C	LEU	A	235	-1.574	10.540	41.849	1.00	10.95
ATOM	788	O	LEU	A	235	-2.066	11.657	41.956	1.00	12.05
ATOM	789	N	PHE	A	236	-0.950	9.892	42.842	1.00	13.16
ATOM	790	CA	PHE	A	236	-0.726	10.459	44.178	1.00	10.40
ATOM	791	CB	PHE	A	236	0.233	9.585	44.996	1.00	14.94
ATOM	792	CG	PHE	A	236	0.599	10.166	46.355	1.00	17.86
ATOM	793	CD1	PHE	A	236	-0.291	10.106	47.423	1.00	19.44
ATOM	794	CE1	PHE	A	236	0.044	10.636	48.668	1.00	20.09
ATOM	795	CZ	PHE	A	236	1.284	11.227	48.859	1.00	19.46
ATOM	796	CE2	PHE	A	236	2.186	11.287	47.809	1.00	19.27
ATOM	797	CD2	PHE	A	236	1.841	10.759	46.565	1.00	19.97
ATOM	798	C	PHE	A	236	-0.156	11.852	44.099	1.00	6.28
ATOM	799	O	PHE	A	236	-0.570	12.726	44.840	1.00	8.31
ATOM	800	N	PHE	A	237	0.799	12.052	43.204	1.00	3.82
ATOM	801	CA	PHE	A	237	1.404	13.353	43.026	1.00	2.00
ATOM	802	CB	PHE	A	237	2.431	13.302	41.927	1.00	2.00
ATOM	803	CG	PHE	A	237	3.076	14.617	41.658	1.00	5.97
ATOM	804	CD1	PHE	A	237	4.224	14.995	42.347	1.00	7.67
ATOM	805	CE1	PHE	A	237	4.842	16.202	42.088	1.00	5.23
ATOM	806	CZ	PHE	A	237	4.310	17.058	41.146	1.00	4.52
ATOM	807	CE2	PHE	A	237	3.166	16.702	40.461	1.00	5.86
ATOM	808	CD2	PHE	A	237	2.547	15.487	40.719	1.00	5.21
ATOM	809	C	PHE	A	237	0.372	14.413	42.695	1.00	2.00
ATOM	810	O	PHE	A	237	0.288	15.421	43.379	1.00	2.15
ATOM	811	N	HIS	A	238	-0.403	14.176	41.642	1.00	4.82
ATOM	812	CA	HIS	A	238	-1.428	15.114	41.174	1.00	8.42
ATOM	813	CB	HIS	A	238	-2.038	14.593	39.882	1.00	8.32
ATOM	814	CG	HIS	A	238	-1.036	14.438	38.794	1.00	9.16
ATOM	815	ND1	HIS	A	238	-0.527	15.513	38.102	1.00	11.04
ATOM	816	CE1	HIS	A	238	0.358	15.085	37.219	1.00	10.69
ATOM	817	NE2	HIS	A	238	0.454	13.772	37.327	1.00	10.36
ATOM	818	CD2	HIS	A	238	-0.399	13.344	38.316	1.00	11.22
ATOM	819	C	HIS	A	238	-2.523	15.362	42.196	1.00	8.33
ATOM	820	O	HIS	A	238	-2.751	16.482	42.620	1.00	9.16
ATOM	821	N	LEU	A	239	-3.196	14.296	42.585	1.00	12.07

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	822	CA	LEU	A	239	-4.176	14.325	43.656	1.00	13.95
ATOM	823	CB	LEU	A	239	-4.564	12.887	44.008	1.00	12.97
ATOM	824	CG	LEU	A	239	-6.041	12.617	44.265	1.00	13.93
ATOM	825	CD1	LEU	A	239	-6.956	13.590	43.540	1.00	10.64
ATOM	826	CD2	LEU	A	239	-6.333	11.202	43.852	1.00	16.40
ATOM	827	C	LEU	A	239	-3.751	15.077	44.930	1.00	13.76
ATOM	828	O	LEU	A	239	-4.594	15.384	45.760	1.00	18.08
ATOM	829	N	SER	A	240	-2.461	15.352	45.102	1.00	11.93
ATOM	830	CA	SER	A	240	-2.009	16.191	46.210	1.00	13.43
ATOM	831	CB	SER	A	240	-0.529	15.952	46.513	1.00	18.66
ATOM	832	OG	SER	A	240	-0.283	14.620	46.909	1.00	24.83
ATOM	833	C	SER	A	240	-2.200	17.664	45.867	1.00	12.02
ATOM	834	O	SER	A	240	-2.536	18.469	46.732	1.00	10.52
ATOM	835	N	ARG	A	241	-1.967	17.983	44.594	1.00	10.21
ATOM	836	CA	ARG	A	241	-1.998	19.328	44.057	1.00	9.84
ATOM	837	CB	ARG	A	241	-1.076	19.410	42.844	1.00	12.11
ATOM	838	CG	ARG	A	241	0.381	19.716	43.172	1.00	17.30
ATOM	839	CD	ARG	A	241	1.402	18.766	42.527	1.00	20.90
ATOM	840	NE	ARG	A	241	2.154	17.955	43.500	1.00	19.01
ATOM	841	CZ	ARG	A	241	3.309	18.320	44.059	1.00	19.63
ATOM	842	NH1	ARG	A	241	3.883	19.494	43.752	1.00	19.40
ATOM	843	NH2	ARG	A	241	3.897	17.500	44.920	1.00	18.01
ATOM	844	C	ARG	A	241	-3.403	19.756	43.655	1.00	14.03
ATOM	845	O	ARG	A	241	-3.767	20.911	43.832	1.00	14.10
ATOM	846	N	GLU	A	242	-4.186	18.832	43.101	1.00	19.47
ATOM	847	CA	GLU	A	242	-5.552	19.135	42.669	1.00	22.54
ATOM	848	CB	GLU	A	242	-5.892	18.440	41.363	1.00	30.13
ATOM	849	CG	GLU	A	242	-4.730	18.361	40.393	1.00	42.01
ATOM	850	CD	GLU	A	242	-4.881	19.313	39.233	1.00	48.30
ATOM	851	OE1	GLU	A	242	-5.932	20.000	39.171	1.00	50.47
ATOM	852	OE2	GLU	A	242	-3.950	19.361	38.387	1.00	53.05
ATOM	853	C	GLU	A	242	-6.555	18.731	43.722	1.00	20.62
ATOM	854	O	GLU	A	242	-7.710	19.133	43.664	1.00	26.70
ATOM	855	N	ARG	A	243	-6.111	17.924	44.672	1.00	15.81
ATOM	856	CA	ARG	A	243	-6.871	17.622	45.882	1.00	14.63
ATOM	857	CB	ARG	A	243	-7.189	18.882	46.684	1.00	16.82
ATOM	858	CG	ARG	A	243	-6.375	18.997	47.982	1.00	22.96
ATOM	859	CD	ARG	A	243	-5.385	20.163	48.033	1.00	21.92
ATOM	860	NE	ARG	A	243	-5.356	20.849	49.332	1.00	24.97
ATOM	861	CZ	ARG	A	243	-5.929	22.033	49.580	1.00	27.07
ATOM	862	NH1	ARG	A	243	-6.595	22.668	48.619	1.00	29.02
ATOM	863	NH2	ARG	A	243	-5.838	22.593	50.786	1.00	24.52
ATOM	864	C	ARG	A	243	-8.108	16.762	45.703	1.00	13.45
ATOM	865	O	ARG	A	243	-8.341	15.892	46.531	1.00	21.66
ATOM	866	N	VAL	A	244	-8.880	16.971	44.637	1.00	8.26
ATOM	867	CA	VAL	A	244	-10.011	16.088	44.277	1.00	5.77
ATOM	868	CB	VAL	A	244	-11.286	16.455	45.077	1.00	2.00
ATOM	869	CG1	VAL	A	244	-11.374	17.915	45.227	1.00	4.93
ATOM	870	CG2	VAL	A	244	-12.541	15.963	44.399	1.00	4.11
ATOM	871	C	VAL	A	244	-10.286	16.096	42.748	1.00	6.46
ATOM	872	O	VAL	A	244	-10.305	17.172	42.139	1.00	7.16
ATOM	873	N	PHE	A	245	-10.480	14.918	42.135	1.00	2.00

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	874	CA	PHE	A	245	-10.780	14.833	40.699	1.00	2.00
ATOM	875	CB	PHE	A	245	-10.310	13.508	40.105	1.00	2.00
ATOM	876	CG	PHE	A	245	-8.821	13.357	40.026	1.00	2.09
ATOM	877	CD1	PHE	A	245	-7.966	14.448	40.238	1.00	2.13
ATOM	878	CE1	PHE	A	245	-6.571	14.303	40.166	1.00	2.00
ATOM	879	CZ	PHE	A	245	-6.030	13.054	39.879	1.00	2.35
ATOM	880	CE2	PHE	A	245	-6.874	11.948	39.649	1.00	2.11
ATOM	881	CD2	PHE	A	245	-8.260	12.106	39.729	1.00	3.36
ATOM	882	C	PHE	A	245	-12.271	14.998	40.372	1.00	4.17
ATOM	883	O	PHE	A	245	-13.155	14.592	41.146	1.00	5.50
ATOM	884	N	SER	A	246	-12.554	15.582	39.211	1.00	2.00
ATOM	885	CA	SER	A	246	-13.912	15.586	38.715	1.00	2.00
ATOM	886	CB	SER	A	246	-14.002	16.351	37.416	1.00	3.48
ATOM	887	OG	SER	A	246	-13.388	15.626	36.369	1.00	6.69
ATOM	888	C	SER	A	246	-14.239	14.154	38.459	1.00	3.42
ATOM	889	O	SER	A	246	-13.352	13.378	38.120	1.00	8.90
ATOM	890	N	GLU	A	247	-15.501	13.790	38.623	1.00	8.83
ATOM	891	CA	GLU	A	247	-15.931	12.424	38.336	1.00	11.81
ATOM	892	CB	GLU	A	247	-17.428	12.265	38.534	1.00	14.51
ATOM	893	CG	GLU	A	247	-17.818	12.126	39.992	1.00	20.39
ATOM	894	CD	GLU	A	247	-19.195	12.685	40.300	1.00	22.98
ATOM	895	OE1	GLU	A	247	-20.079	12.623	39.409	1.00	24.75
ATOM	896	OE2	GLU	A	247	-19.388	13.173	41.443	1.00	23.79
ATOM	897	C	GLU	A	247	-15.542	12.043	36.923	1.00	13.67
ATOM	898	O	GLU	A	247	-15.065	10.945	36.693	1.00	11.40
ATOM	899	N	ASP	A	248	-15.710	12.972	35.986	1.00	20.80
ATOM	900	CA	ASP	A	248	-15.310	12.735	34.603	1.00	27.14
ATOM	901	CB	ASP	A	248	-15.789	13.862	33.678	1.00	33.47
ATOM	902	CG	ASP	A	248	-16.577	13.336	32.468	1.00	41.51
ATOM	903	OD1	ASP	A	248	-17.114	14.184	31.709	1.00	44.30
ATOM	904	OD2	ASP	A	248	-16.712	12.104	32.195	1.00	42.84
ATOM	905	C	ASP	A	248	-13.804	12.457	34.438	1.00	26.38
ATOM	906	O	ASP	A	248	-13.402	11.775	33.492	1.00	27.22
ATOM	907	N	ARG	A	249	-12.982	12.973	35.356	1.00	23.02
ATOM	908	CA	ARG	A	249	-11.557	12.671	35.338	1.00	18.30
ATOM	909	CB	ARG	A	249	-10.719	13.771	35.989	1.00	21.33
ATOM	910	CG	ARG	A	249	-9.210	13.504	35.948	1.00	26.93
ATOM	911	CD	ARG	A	249	-8.307	14.713	36.270	1.00	30.97
ATOM	912	NE	ARG	A	249	-6.894	14.318	36.364	1.00	31.18
ATOM	913	CZ	ARG	A	249	-5.902	15.117	36.763	1.00	33.25
ATOM	914	NH1	ARG	A	249	-6.139	16.376	37.124	1.00	32.63
ATOM	915	NH2	ARG	A	249	-4.657	14.653	36.797	1.00	33.88
ATOM	916	C	ARG	A	249	-11.310	11.341	36.014	1.00	15.86
ATOM	917	O	ARG	A	249	-10.461	10.582	35.566	1.00	17.48
ATOM	918	N	ALA	A	250	-12.049	11.046	37.081	1.00	11.34
ATOM	919	CA	ALA	A	250	-11.860	9.773	37.779	1.00	10.56
ATOM	920	CB	ALA	A	250	-12.478	9.796	39.150	1.00	7.55
ATOM	921	C	ALA	A	250	-12.433	8.641	36.960	1.00	12.21
ATOM	922	O	ALA	A	250	-11.911	7.536	36.975	1.00	13.09
ATOM	923	N	ARG	A	251	-13.513	8.934	36.243	1.00	16.78
ATOM	924	CA	ARG	A	251	-14.131	7.984	35.326	1.00	18.77
ATOM	925	CB	ARG	A	251	-15.262	8.657	34.547	1.00	20.30

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	926	CG	ARG	A	251	-16.267	7.733	33.894	1.00	21.32
ATOM	927	CD	ARG	A	251	-17.293	8.481	33.035	1.00	26.36
ATOM	928	NE	ARG	A	251	-17.956	9.566	33.763	1.00	29.99
ATOM	929	CZ	ARG	A	251	-18.696	9.404	34.869	1.00	32.84
ATOM	930	NH1	ARG	A	251	-18.877	8.187	35.382	1.00	31.79
ATOM	931	NH2	ARG	A	251	-19.257	10.463	35.470	1.00	31.78
ATOM	932	C	ARG	A	251	-13.046	7.514	34.381	1.00	18.69
ATOM	933	O	ARG	A	251	-12.886	6.313	34.179	1.00	21.73
ATOM	934	N	PHE	A	252	-12.277	8.465	33.848	1.00	14.28
ATOM	935	CA	PHE	A	252	-11.204	8.152	32.919	1.00	11.87
ATOM	936	CB	PHE	A	252	-10.573	9.414	32.341	1.00	13.19
ATOM	937	CG	PHE	A	252	-9.379	9.132	31.496	1.00	15.31
ATOM	938	CD1	PHE	A	252	-9.521	8.802	30.164	1.00	19.60
ATOM	939	CE1	PHE	A	252	-8.410	8.506	29.385	1.00	22.22
ATOM	940	CZ	PHE	A	252	-7.143	8.528	29.947	1.00	20.67
ATOM	941	CE2	PHE	A	252	-6.997	8.842	31.271	1.00	20.37
ATOM	942	CD2	PHE	A	252	-8.115	9.132	32.042	1.00	17.82
ATOM	943	C	PHE	A	252	-10.099	7.253	33.491	1.00	10.80
ATOM	944	O	PHE	A	252	-9.635	6.349	32.805	1.00	13.98
ATOM	945	N	TYR	A	253	-9.653	7.507	34.717	1.00	5.62
ATOM	946	CA	TYR	A	253	-8.592	6.691	35.278	1.00	2.59
ATOM	947	CB	TYR	A	253	-7.932	7.381	36.459	1.00	2.00
ATOM	948	CG	TYR	A	253	-7.201	8.630	36.052	1.00	2.22
ATOM	949	CD1	TYR	A	253	-6.435	8.667	34.884	1.00	2.00
ATOM	950	CE1	TYR	A	253	-5.774	9.820	34.490	1.00	2.00
ATOM	951	CZ	TYR	A	253	-5.877	10.966	35.260	1.00	4.68
ATOM	952	OH	TYR	A	253	-5.219	12.119	34.887	1.00	5.21
ATOM	953	CE2	TYR	A	253	-6.634	10.961	36.432	1.00	7.42
ATOM	954	CD2	TYR	A	253	-7.290	9.790	36.820	1.00	5.43
ATOM	955	C	TYR	A	253	-9.128	5.326	35.660	1.00	6.96
ATOM	956	O	TYR	A	253	-8.486	4.304	35.397	1.00	9.53
ATOM	957	N	GLY	A	254	-10.324	5.317	36.248	1.00	9.33
ATOM	958	CA	GLY	A	254	-10.981	4.100	36.693	1.00	7.25
ATOM	959	C	GLY	A	254	-11.173	3.127	35.555	1.00	8.88
ATOM	960	O	GLY	A	254	-10.852	1.945	35.693	1.00	7.60
ATOM	961	N	ALA	A	255	-11.675	3.639	34.428	1.00	10.17
ATOM	962	CA	ALA	A	255	-11.881	2.850	33.206	1.00	7.78
ATOM	963	CB	ALA	A	255	-12.416	3.713	32.084	1.00	3.52
ATOM	964	C	ALA	A	255	-10.594	2.178	32.778	1.00	7.86
ATOM	965	O	ALA	A	255	-10.574	0.972	32.517	1.00	8.42
ATOM	966	N	GLU	A	256	-9.512	2.950	32.733	1.00	7.56
ATOM	967	CA	GLU	A	256	-8.230	2.377	32.353	1.00	10.01
ATOM	968	CB	GLU	A	256	-7.199	3.457	32.059	1.00	11.01
ATOM	969	CG	GLU	A	256	-7.545	4.199	30.781	1.00	19.08
ATOM	970	CD	GLU	A	256	-6.481	5.175	30.310	1.00	24.92
ATOM	971	OE1	GLU	A	256	-5.593	5.559	31.111	1.00	28.83
ATOM	972	OE2	GLU	A	256	-6.545	5.565	29.121	1.00	25.17
ATOM	973	C	GLU	A	256	-7.744	1.345	33.368	1.00	9.76
ATOM	974	O	GLU	A	256	-7.340	0.257	32.988	1.00	13.11
ATOM	975	N	ILE	A	257	-7.828	1.653	34.653	1.00	7.54
ATOM	976	CA	ILE	A	257	-7.418	0.691	35.662	1.00	7.64
ATOM	977	CB	ILE	A	257	-7.542	1.315	37.059	1.00	11.05

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	978	CG1	ILE	A	257	-6.443	2.378	37.227	1.00	12.52
ATOM	979	CD1	ILE	A	257	-6.872	3.595	37.959	1.00	10.73
ATOM	980	CG2	ILE	A	257	-7.479	0.239	38.153	1.00	8.70
ATOM	981	C	ILE	A	257	-8.216	-0.606	35.528	1.00	8.16
ATOM	982	O	ILE	A	257	-7.633	-1.696	35.466	1.00	7.37
ATOM	983	N	VAL	A	258	-9.541	-0.477	35.441	1.00	9.01
ATOM	984	CA	VAL	A	258	-10.429	-1.631	35.268	1.00	7.18
ATOM	985	CB	VAL	A	258	-11.902	-1.241	35.119	1.00	2.93
ATOM	986	CG1	VAL	A	258	-12.702	-2.442	34.690	1.00	2.00
ATOM	987	CG2	VAL	A	258	-12.443	-0.704	36.420	1.00	2.00
ATOM	988	C	VAL	A	258	-10.025	-2.461	34.061	1.00	8.66
ATOM	989	O	VAL	A	258	-9.829	-3.673	34.189	1.00	10.98
ATOM	990	N	SER	A	259	-9.895	-1.811	32.905	1.00	6.46
ATOM	991	CA	SER	A	259	-9.383	-2.479	31.713	1.00	8.54
ATOM	992	CB	SER	A	259	-9.007	-1.478	30.620	1.00	11.72
ATOM	993	OG	SER	A	259	-8.323	-2.138	29.557	1.00	14.31
ATOM	994	C	SER	A	259	-8.160	-3.321	32.036	1.00	7.89
ATOM	995	O	SER	A	259	-8.147	-4.516	31.797	1.00	11.33
ATOM	996	N	ALA	A	260	-7.142	-2.687	32.594	1.00	6.11
ATOM	997	CA	ALA	A	260	-5.876	-3.338	32.824	1.00	5.59
ATOM	998	CB	ALA	A	260	-4.876	-2.352	33.368	1.00	5.91
ATOM	999	C	ALA	A	260	-6.031	-4.520	33.759	1.00	8.69
ATOM	1000	O	ALA	A	260	-5.489	-5.595	33.464	1.00	10.96
ATOM	1001	N	LEU	A	261	-6.767	-4.328	34.863	1.00	5.59
ATOM	1002	CA	LEU	A	261	-6.969	-5.387	35.856	1.00	7.05
ATOM	1003	CB	LEU	A	261	-7.781	-4.889	37.047	1.00	7.02
ATOM	1004	CG	LEU	A	261	-7.135	-3.979	38.088	1.00	9.71
ATOM	1005	CD1	LEU	A	261	-8.208	-3.459	39.027	1.00	8.51
ATOM	1006	CD2	LEU	A	261	-6.009	-4.660	38.872	1.00	7.95
ATOM	1007	C	LEU	A	261	-7.723	-6.547	35.235	1.00	9.57
ATOM	1008	O	LEU	A	261	-7.393	-7.722	35.440	1.00	10.43
ATOM	1009	N	ASP	A	262	-8.756	-6.200	34.478	1.00	10.73
ATOM	1010	CA	ASP	A	262	-9.573	-7.188	33.799	1.00	12.07
ATOM	1011	CB	ASP	A	262	-10.561	-6.493	32.856	1.00	11.69
ATOM	1012	CG	ASP	A	262	-11.169	-7.440	31.858	1.00	11.58
ATOM	1013	OD1	ASP	A	262	-11.173	-7.117	30.646	1.00	9.76
ATOM	1014	OD2	ASP	A	262	-11.654	-8.537	32.206	1.00	14.40
ATOM	1015	C	ASP	A	262	-8.671	-8.135	33.022	1.00	11.58
ATOM	1016	O	ASP	A	262	-8.883	-9.349	33.023	1.00	13.83
ATOM	1017	N	TYR	A	263	-7.660	-7.562	32.372	1.00	9.31
ATOM	1018	CA	TYR	A	263	-6.749	-8.306	31.519	1.00	6.69
ATOM	1019	CB	TYR	A	263	-5.926	-7.343	30.663	1.00	5.18
ATOM	1020	CG	TYR	A	263	-4.620	-7.885	30.157	1.00	5.20
ATOM	1021	CD1	TYR	A	263	-4.578	-8.776	29.104	1.00	3.18
ATOM	1022	CE1	TYR	A	263	-3.378	-9.273	28.640	1.00	3.93
ATOM	1023	CZ	TYR	A	263	-2.198	-8.865	29.219	1.00	5.10
ATOM	1024	OH	TYR	A	263	-1.002	-9.365	28.762	1.00	8.97
ATOM	1025	CE2	TYR	A	263	-2.207	-7.972	30.259	1.00	6.12
ATOM	1026	CD2	TYR	A	263	-3.416	-7.489	30.729	1.00	8.30
ATOM	1027	C	TYR	A	263	-5.877	-9.195	32.380	1.00	7.87
ATOM	1028	O	TYR	A	263	-5.690	-10.357	32.063	1.00	11.02
ATOM	1029	N	LEU	A	264	-5.373	-8.653	33.483	1.00	6.46

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1030	CA	LEU	A	264	-4.626	-9.437	34.455	1.00	3.11
ATOM	1031	CB	LEU	A	264	-4.174	-8.559	35.623	1.00	3.56
ATOM	1032	CG	LEU	A	264	-3.016	-7.591	35.355	1.00	3.38
ATOM	1033	CD1	LEU	A	264	-2.798	-6.686	36.564	1.00	2.00
ATOM	1034	CD2	LEU	A	264	-1.741	-8.350	34.956	1.00	2.00
ATOM	1035	C	LEU	A	264	-5.460	-10.606	34.968	1.00	3.11
ATOM	1036	O	LEU	A	264	-5.038	-11.766	34.874	1.00	5.05
ATOM	1037	N	HIS	A	265	-6.646	-10.310	35.493	1.00	2.00
ATOM	1038	CA	HIS	A	265	-7.544	-11.354	35.989	1.00	2.00
ATOM	1039	CB	HIS	A	265	-8.853	-10.736	36.443	1.00	3.27
ATOM	1040	CG	HIS	A	265	-8.749	-9.974	37.722	1.00	7.09
ATOM	1041	ND1	HIS	A	265	-9.858	-9.550	38.424	1.00	7.78
ATOM	1042	CE1	HIS	A	265	-9.466	-8.906	39.509	1.00	8.06
ATOM	1043	NE2	HIS	A	265	-8.144	-8.889	39.532	1.00	8.28
ATOM	1044	CD2	HIS	A	265	-7.671	-9.560	38.431	1.00	7.75
ATOM	1045	C	HIS	A	265	-7.810	-12.430	34.932	1.00	2.00
ATOM	1046	O	HIS	A	265	-7.794	-13.618	35.218	1.00	2.00
ATOM	1047	N	SER	A	266	-8.037	-11.981	33.704	1.00	3.00
ATOM	1048	CA	SER	A	266	-8.193	-12.842	32.545	1.00	3.05
ATOM	1049	CB	SER	A	266	-8.362	-11.975	31.300	1.00	2.18
ATOM	1050	OG	SER	A	266	-7.309	-12.193	30.382	1.00	2.00
ATOM	1051	C	SER	A	266	-7.026	-13.816	32.350	1.00	4.19
ATOM	1052	O	SER	A	266	-7.239	-14.954	31.946	1.00	2.17
ATOM	1053	N	ARG	A	267	-5.804	-13.348	32.619	1.00	7.93
ATOM	1054	CA	ARG	A	267	-4.597	-14.168	32.520	1.00	9.33
ATOM	1055	CB	ARG	A	267	-3.456	-13.402	31.863	1.00	7.77
ATOM	1056	CG	ARG	A	267	-3.908	-12.468	30.772	1.00	15.83
ATOM	1057	CD	ARG	A	267	-3.423	-12.808	29.368	1.00	22.54
ATOM	1058	NE	ARG	A	267	-2.002	-12.512	29.248	1.00	27.49
ATOM	1059	CZ	ARG	A	267	-1.127	-13.290	28.631	1.00	31.28
ATOM	1060	NH1	ARG	A	267	-1.519	-14.419	28.036	1.00	31.45
ATOM	1061	NH2	ARG	A	267	0.150	-12.933	28.607	1.00	33.16
ATOM	1062	C	ARG	A	267	-4.184	-14.677	33.898	1.00	13.33
ATOM	1063	O	ARG	A	267	-3.032	-15.060	34.112	1.00	17.32
ATOM	1064	N	ASP	A	268	-5.137	-14.673	34.828	1.00	13.39
ATOM	1065	CA	ASP	A	268	-5.019	-15.386	36.101	1.00	14.93
ATOM	1066	CB	ASP	A	268	-4.564	-16.836	35.883	1.00	17.33
ATOM	1067	CG	ASP	A	268	-5.612	-17.689	35.166	1.00	22.64
ATOM	1068	OD1	ASP	A	268	-6.561	-17.127	34.576	1.00	24.96
ATOM	1069	OD2	ASP	A	268	-5.560	-18.940	35.129	1.00	24.99
ATOM	1070	C	ASP	A	268	-4.139	-14.714	37.151	1.00	15.41
ATOM	1071	O	ASP	A	268	-3.770	-15.340	38.150	1.00	18.69
ATOM	1072	N	VAL	A	269	-3.833	-13.437	36.945	1.00	10.02
ATOM	1073	CA	VAL	A	269	-2.963	-12.720	37.858	1.00	6.59
ATOM	1074	CB	VAL	A	269	-1.947	-11.853	37.103	1.00	7.45
ATOM	1075	CG1	VAL	A	269	-1.006	-11.136	38.078	1.00	7.11
ATOM	1076	CG2	VAL	A	269	-1.162	-12.686	36.073	1.00	5.78
ATOM	1077	C	VAL	A	269	-3.820	-11.807	38.673	1.00	7.01
ATOM	1078	O	VAL	A	269	-4.675	-11.128	38.117	1.00	7.24
ATOM	1079	N	VAL	A	270	-3.600	-11.793	39.989	1.00	9.82
ATOM	1080	CA	VAL	A	270	-4.199	-10.778	40.865	1.00	10.76
ATOM	1081	CB	VAL	A	270	-4.728	-11.355	42.156	1.00	9.09

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1082	CG1	VAL	A	270	-5.448	-10.269	42.923	1.00	6.31
ATOM	1083	CG2	VAL	A	270	-5.645	-12.506	41.876	1.00	10.51
ATOM	1084	C	VAL	A	270	-3.165	-9.747	41.259	1.00	13.99
ATOM	1085	O	VAL	A	270	-2.072	-10.109	41.701	1.00	17.06
ATOM	1086	N	TYR	A	271	-3.520	-8.469	41.130	1.00	15.45
ATOM	1087	CA	TYR	A	271	-2.553	-7.386	41.287	1.00	15.75
ATOM	1088	CB	TYR	A	271	-3.044	-6.104	40.651	1.00	15.96
ATOM	1089	CG	TYR	A	271	-2.044	-4.990	40.763	1.00	17.33
ATOM	1090	CD1	TYR	A	271	-0.853	-5.020	40.032	1.00	16.87
ATOM	1091	CE1	TYR	A	271	0.069	-3.999	40.135	1.00	17.14
ATOM	1092	CZ	TYR	A	271	-0.195	-2.929	40.982	1.00	19.63
ATOM	1093	OH	TYR	A	271	0.712	-1.897	41.097	1.00	22.51
ATOM	1094	CE2	TYR	A	271	-1.366	-2.879	41.713	1.00	18.04
ATOM	1095	CD2	TYR	A	271	-2.280	-3.907	41.604	1.00	18.02
ATOM	1096	C	TYR	A	271	-2.180	-7.139	42.733	1.00	16.74
ATOM	1097	O	TYR	A	271	-1.011	-7.237	43.090	1.00	20.28
ATOM	1098	N	ARG	A	272	-3.168	-6.801	43.552	1.00	17.70
ATOM	1099	CA	ARG	A	272	-3.025	-6.850	45.013	1.00	19.65
ATOM	1100	CB	ARG	A	272	-2.211	-8.071	45.457	1.00	16.16
ATOM	1101	CG	ARG	A	272	-2.992	-9.362	45.456	1.00	14.21
ATOM	1102	CD	ARG	A	272	-2.515	-10.347	46.493	1.00	12.14
ATOM	1103	NE	ARG	A	272	-1.206	-10.902	46.150	1.00	8.20
ATOM	1104	CZ	ARG	A	272	-0.507	-11.709	46.933	1.00	4.92
ATOM	1105	NH1	ARG	A	272	-0.983	-12.049	48.125	1.00	5.63
ATOM	1106	NH2	ARG	A	272	0.668	-12.175	46.528	1.00	2.00
ATOM	1107	C	ARG	A	272	-2.440	-5.629	45.682	1.00	21.67
ATOM	1108	O	ARG	A	272	-2.510	-5.522	46.896	1.00	27.94
ATOM	1109	N	ASP	A	273	-1.863	-4.708	44.924	1.00	21.64
ATOM	1110	CA	ASP	A	273	-1.301	-3.528	45.556	1.00	22.15
ATOM	1111	CB	ASP	A	273	0.222	-3.565	45.499	1.00	28.08
ATOM	1112	CG	ASP	A	273	0.876	-2.895	46.720	1.00	32.52
ATOM	1113	OD1	ASP	A	273	0.151	-2.595	47.702	1.00	29.10
ATOM	1114	OD2	ASP	A	273	2.109	-2.631	46.770	1.00	34.26
ATOM	1115	C	ASP	A	273	-1.826	-2.217	44.995	1.00	21.77
ATOM	1116	O	ASP	A	273	-1.147	-1.197	45.045	1.00	27.34
ATOM	1117	N	LEU	A	274	-3.045	-2.228	44.481	1.00	17.73
ATOM	1118	CA	LEU	A	274	-3.610	-1.039	43.857	1.00	13.92
ATOM	1119	CB	LEU	A	274	-5.030	-1.340	43.422	1.00	9.76
ATOM	1120	CG	LEU	A	274	-5.506	-0.521	42.242	1.00	9.33
ATOM	1121	CD1	LEU	A	274	-5.396	-1.276	40.910	1.00	8.23
ATOM	1122	CD2	LEU	A	274	-6.916	-0.159	42.533	1.00	7.44
ATOM	1123	C	LEU	A	274	-3.574	0.191	44.770	1.00	14.88
ATOM	1124	O	LEU	A	274	-4.129	0.173	45.866	1.00	19.59
ATOM	1125	N	LYS	A	275	-2.885	1.242	44.338	1.00	13.47
ATOM	1126	CA	LYS	A	275	-2.859	2.502	45.089	1.00	13.09
ATOM	1127	CB	LYS	A	275	-1.982	2.409	46.341	1.00	11.39
ATOM	1128	CG	LYS	A	275	-0.514	2.086	46.149	1.00	14.33
ATOM	1129	CD	LYS	A	275	0.214	2.351	47.509	1.00	18.51
ATOM	1130	CE	LYS	A	275	1.668	1.825	47.603	1.00	15.35
ATOM	1131	NZ	LYS	A	275	1.714	0.330	47.725	1.00	12.90
ATOM	1132	C	LYS	A	275	-2.466	3.691	44.228	1.00	12.82
ATOM	1133	O	LYS	A	275	-2.066	3.530	43.087	1.00	14.18

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1134	N	LEU	A	276	-2.581	4.891	44.773	1.00	12.66
ATOM	1135	CA	LEU	A	276	-2.217	6.086	44.018	1.00	13.20
ATOM	1136	CB	LEU	A	276	-2.515	7.339	44.833	1.00	13.28
ATOM	1137	CG	LEU	A	276	-3.996	7.426	45.204	1.00	15.59
ATOM	1138	CD1	LEU	A	276	-4.274	8.695	45.946	1.00	17.83
ATOM	1139	CD2	LEU	A	276	-4.859	7.352	43.966	1.00	16.71
ATOM	1140	C	LEU	A	276	-0.760	6.066	43.572	1.00	12.67
ATOM	1141	O	LEU	A	276	-0.423	6.524	42.480	1.00	14.01
ATOM	1142	N	GLU	A	277	0.091	5.502	44.415	1.00	11.30
ATOM	1143	CA	GLU	A	277	1.515	5.512	44.187	1.00	12.17
ATOM	1144	CB	GLU	A	277	2.255	5.088	45.453	1.00	17.18
ATOM	1145	CG	GLU	A	277	2.294	6.164	46.524	1.00	21.52
ATOM	1146	CD	GLU	A	277	1.163	6.032	47.528	1.00	26.98
ATOM	1147	OE1	GLU	A	277	0.005	5.717	47.132	1.00	31.14
ATOM	1148	OE2	GLU	A	277	1.427	6.249	48.729	1.00	28.95
ATOM	1149	C	GLU	A	277	1.886	4.588	43.062	1.00	12.72
ATOM	1150	O	GLU	A	277	2.935	4.737	42.463	1.00	16.01
ATOM	1151	N	ASN	A	278	1.044	3.612	42.778	1.00	14.09
ATOM	1152	CA	ASN	A	278	1.409	2.626	41.777	1.00	16.17
ATOM	1153	CB	ASN	A	278	1.057	1.195	42.242	1.00	18.41
ATOM	1154	CG	ASN	A	278	1.947	0.682	43.398	1.00	19.23
ATOM	1155	OD1	ASN	A	278	2.901	1.333	43.827	1.00	24.41
ATOM	1156	ND2	ASN	A	278	1.630	-0.503	43.890	1.00	16.64
ATOM	1157	C	ASN	A	278	0.728	2.954	40.460	1.00	17.72
ATOM	1158	O	ASN	A	278	0.825	2.188	39.505	1.00	26.88
ATOM	1159	N	LEU	A	279	0.022	4.081	40.406	1.00	12.26
ATOM	1160	CA	LEU	A	279	-0.675	4.457	39.188	1.00	7.30
ATOM	1161	CB	LEU	A	279	-2.116	4.815	39.480	1.00	2.00
ATOM	1162	CG	LEU	A	279	-2.939	3.709	40.111	1.00	2.00
ATOM	1163	CD1	LEU	A	279	-4.289	4.233	40.586	1.00	4.54
ATOM	1164	CD2	LEU	A	279	-3.121	2.567	39.158	1.00	2.00
ATOM	1165	C	LEU	A	279	0.020	5.630	38.547	1.00	12.00
ATOM	1166	O	LEU	A	279	-0.048	6.754	39.054	1.00	15.43
ATOM	1167	N	MET	A	280	0.684	5.364	37.428	1.00	11.29
ATOM	1168	CA	MET	A	280	1.426	6.383	36.702	1.00	10.05
ATOM	1169	CB	MET	A	280	2.675	5.771	36.076	1.00	15.79
ATOM	1170	CG	MET	A	280	3.545	4.985	37.024	1.00	21.72
ATOM	1171	SD	MET	A	280	3.754	5.819	38.584	1.00	27.06
ATOM	1172	CE	MET	A	280	5.330	6.743	38.254	1.00	25.39
ATOM	1173	C	MET	A	280	0.611	7.012	35.592	1.00	8.61
ATOM	1174	O	MET	A	280	-0.538	6.633	35.345	1.00	11.31
ATOM	1175	N	LEU	A	281	1.239	7.974	34.925	1.00	5.78
ATOM	1176	CA	LEU	A	281	0.717	8.629	33.740	1.00	2.07
ATOM	1177	CB	LEU	A	281	0.226	10.043	34.084	1.00	2.00
ATOM	1178	CG	LEU	A	281	-0.979	10.338	34.991	1.00	2.00
ATOM	1179	CD1	LEU	A	281	-1.417	11.771	34.784	1.00	2.87
ATOM	1180	CD2	LEU	A	281	-2.153	9.397	34.746	1.00	2.12
ATOM	1181	C	LEU	A	281	1.840	8.722	32.707	1.00	3.99
ATOM	1182	O	LEU	A	281	2.905	9.292	32.969	1.00	2.00
ATOM	1183	N	ASP	A	282	1.606	8.154	31.530	1.00	7.30
ATOM	1184	CA	ASP	A	282	2.572	8.239	30.438	1.00	8.52
ATOM	1185	CB	ASP	A	282	2.296	7.167	29.383	1.00	13.73

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1186	CG	ASP	A	282	0.896	7.247	28.818	1.00	16.68
ATOM	1187	OD1	ASP	A	282	0.155	8.168	29.231	1.00	18.36
ATOM	1188	OD2	ASP	A	282	0.459	6.438	27.958	1.00	18.90
ATOM	1189	C	ASP	A	282	2.582	9.624	29.806	1.00	5.65
ATOM	1190	O	ASP	A	282	1.868	10.521	30.254	1.00	2.00
ATOM	1191	N	LYS	A	283	3.397	9.783	28.764	1.00	8.25
ATOM	1192	CA	LYS	A	283	3.570	11.088	28.116	1.00	13.57
ATOM	1193	CB	LYS	A	283	4.632	11.042	27.001	1.00	16.92
ATOM	1194	CG	LYS	A	283	4.568	9.841	26.044	1.00	20.42
ATOM	1195	CD	LYS	A	283	5.386	10.106	24.759	1.00	22.50
ATOM	1196	CE	LYS	A	283	6.739	9.370	24.746	1.00	22.07
ATOM	1197	NZ	LYS	A	283	7.521	9.612	23.497	1.00	20.59
ATOM	1198	C	LYS	A	283	2.261	11.702	27.606	1.00	12.66
ATOM	1199	O	LYS	A	283	2.051	12.912	27.694	1.00	13.40
ATOM	1200	N	ASP	A	284	1.375	10.861	27.098	1.00	11.64
ATOM	1201	CA	ASP	A	284	0.130	11.348	26.551	1.00	13.33
ATOM	1202	CB	ASP	A	284	-0.238	10.561	25.282	1.00	18.18
ATOM	1203	CG	ASP	A	284	0.540	11.050	24.035	1.00	22.64
ATOM	1204	OD1	ASP	A	284	0.433	12.255	23.684	1.00	22.92
ATOM	1205	OD2	ASP	A	284	1.287	10.309	23.347	1.00	22.09
ATOM	1206	C	ASP	A	284	-1.007	11.408	27.577	1.00	12.90
ATOM	1207	O	ASP	A	284	-2.085	11.877	27.258	1.00	17.88
ATOM	1208	N	GLY	A	285	-0.768	10.948	28.803	1.00	12.91
ATOM	1209	CA	GLY	A	285	-1.712	11.141	29.897	1.00	10.52
ATOM	1210	C	GLY	A	285	-2.604	9.978	30.304	1.00	11.06
ATOM	1211	O	GLY	A	285	-3.496	10.150	31.133	1.00	10.20
ATOM	1212	N	HIS	A	286	-2.374	8.803	29.723	1.00	11.24
ATOM	1213	CA	HIS	A	286	-3.127	7.586	30.060	1.00	9.81
ATOM	1214	CB	HIS	A	286	-3.158	6.608	28.870	1.00	11.11
ATOM	1215	CG	HIS	A	286	-3.807	7.171	27.641	1.00	11.60
ATOM	1216	ND1	HIS	A	286	-5.100	6.858	27.269	1.00	11.62
ATOM	1217	CE1	HIS	A	286	-5.409	7.508	26.163	1.00	7.93
ATOM	1218	NE2	HIS	A	286	-4.363	8.228	25.800	1.00	9.43
ATOM	1219	CD2	HIS	A	286	-3.351	8.042	26.712	1.00	9.35
ATOM	1220	C	HIS	A	286	-2.525	6.886	31.267	1.00	8.93
ATOM	1221	O	HIS	A	286	-1.361	7.099	31.610	1.00	9.27
ATOM	1222	N	ILE	A	287	-3.313	6.032	31.902	1.00	7.87
ATOM	1223	CA	ILE	A	287	-2.827	5.302	33.051	1.00	8.76
ATOM	1224	CB	ILE	A	287	-3.968	4.595	33.752	1.00	10.57
ATOM	1225	CG1	ILE	A	287	-4.696	5.589	34.672	1.00	13.11
ATOM	1226	CD1	ILE	A	287	-4.281	5.553	36.135	1.00	11.59
ATOM	1227	CG2	ILE	A	287	-3.458	3.343	34.507	1.00	12.90
ATOM	1228	C	ILE	A	287	-1.743	4.313	32.685	1.00	9.76
ATOM	1229	O	ILE	A	287	-1.724	3.757	31.594	1.00	12.23
ATOM	1230	N	LYS	A	288	-0.821	4.133	33.616	1.00	13.88
ATOM	1231	CA	LYS	A	288	0.144	3.058	33.578	1.00	15.36
ATOM	1232	CB	LYS	A	288	1.514	3.603	33.215	1.00	16.11
ATOM	1233	CG	LYS	A	288	1.690	3.861	31.735	1.00	23.75
ATOM	1234	CD	LYS	A	288	1.420	2.607	30.903	1.00	27.10
ATOM	1235	CE	LYS	A	288	1.929	2.776	29.473	1.00	28.84
ATOM	1236	NZ	LYS	A	288	1.853	1.488	28.709	1.00	30.01
ATOM	1237	C	LYS	A	288	0.171	2.512	34.982	1.00	17.26

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1238	O	LYS	A	288	0.488	3.255	35.918	1.00	21.27
ATOM	1239	N	ILE	A	289	-0.202	1.246	35.156	1.00	13.63
ATOM	1240	CA	ILE	A	289	0.007	0.593	36.446	1.00	10.47
ATOM	1241	CB	ILE	A	289	-0.947	-0.574	36.627	1.00	9.99
ATOM	1242	CG1	ILE	A	289	-2.383	-0.088	36.750	1.00	12.51
ATOM	1243	CD1	ILE	A	289	-3.384	-1.240	36.977	1.00	15.02
ATOM	1244	CG2	ILE	A	289	-0.558	-1.394	37.835	1.00	6.59
ATOM	1245	C	ILE	A	289	1.434	0.073	36.493	1.00	8.91
ATOM	1246	O	ILE	A	289	1.844	-0.672	35.617	1.00	11.53
ATOM	1247	N	THR	A	290	2.192	0.468	37.504	1.00	7.24
ATOM	1248	CA	THR	A	290	3.470	-0.173	37.783	1.00	11.92
ATOM	1249	CB	THR	A	290	4.590	0.856	37.617	1.00	13.73
ATOM	1250	OG1	THR	A	290	5.845	0.292	38.048	1.00	19.87
ATOM	1251	CG2	THR	A	290	4.352	2.029	38.545	1.00	13.69
ATOM	1252	C	THR	A	290	3.523	-0.875	39.177	1.00	13.06
ATOM	1253	O	THR	A	290	2.631	-0.696	40.015	1.00	13.14
ATOM	1254	N	ASP	A	291	4.558	-1.682	39.408	1.00	10.41
ATOM	1255	CA	ASP	A	291	4.841	-2.217	40.743	1.00	10.96
ATOM	1256	CB	ASP	A	291	4.495	-1.194	41.837	1.00	8.28
ATOM	1257	CG	ASP	A	291	5.087	-1.540	43.199	1.00	6.40
ATOM	1258	OD1	ASP	A	291	6.051	-2.329	43.278	1.00	5.88
ATOM	1259	OD2	ASP	A	291	4.644	-1.052	44.259	1.00	4.36
ATOM	1260	C	ASP	A	291	4.139	-3.543	40.973	1.00	13.95
ATOM	1261	O	ASP	A	291	3.074	-3.604	41.581	1.00	19.80
ATOM	1262	N	PHE	A	292	4.765	-4.613	40.498	1.00	14.16
ATOM	1263	CA	PHE	A	292	4.135	-5.924	40.494	1.00	11.92
ATOM	1264	CB	PHE	A	292	4.229	-6.536	39.090	1.00	9.29
ATOM	1265	CG	PHE	A	292	3.561	-5.704	38.042	1.00	8.89
ATOM	1266	CD1	PHE	A	292	4.306	-4.918	37.185	1.00	8.76
ATOM	1267	CE1	PHE	A	292	3.683	-4.130	36.216	1.00	7.86
ATOM	1268	CZ	PHE	A	292	2.302	-4.106	36.115	1.00	6.05
ATOM	1269	CE2	PHE	A	292	1.546	-4.871	36.979	1.00	9.27
ATOM	1270	CD2	PHE	A	292	2.175	-5.665	37.944	1.00	9.42
ATOM	1271	C	PHE	A	292	4.707	-6.838	41.560	1.00	11.39
ATOM	1272	O	PHE	A	292	4.599	-8.065	41.468	1.00	13.14
ATOM	1273	N	GLY	A	293	5.314	-6.228	42.575	1.00	11.27
ATOM	1274	CA	GLY	A	293	5.857	-6.954	43.716	1.00	11.03
ATOM	1275	C	GLY	A	293	4.880	-7.961	44.300	1.00	9.86
ATOM	1276	O	GLY	A	293	5.222	-9.117	44.496	1.00	10.07
ATOM	1277	N	LEU	A	294	3.641	-7.537	44.513	1.00	10.59
ATOM	1278	CA	LEU	A	294	2.691	-8.381	45.194	1.00	12.73
ATOM	1279	CB	LEU	A	294	1.968	-7.568	46.264	1.00	11.55
ATOM	1280	CG	LEU	A	294	2.833	-6.822	47.275	1.00	9.66
ATOM	1281	CD1	LEU	A	294	1.913	-6.303	48.321	1.00	11.57
ATOM	1282	CD2	LEU	A	294	3.887	-7.701	47.908	1.00	9.53
ATOM	1283	C	LEU	A	294	1.695	-9.144	44.308	1.00	18.57
ATOM	1284	O	LEU	A	294	0.727	-9.711	44.818	1.00	24.42
ATOM	1285	N	CYS	A	295	1.928	-9.189	42.999	1.00	20.56
ATOM	1286	CA	CYS	A	295	1.118	-10.034	42.114	1.00	19.93
ATOM	1287	CB	CYS	A	295	1.634	-9.957	40.696	1.00	23.56
ATOM	1288	SG	CYS	A	295	1.191	-8.392	39.972	1.00	39.04
ATOM	1289	C	CYS	A	295	1.120	-11.488	42.527	1.00	16.76

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1290	O	CYS	A	295	2.152	-12.019	42.918	1.00	19.03
ATOM	1291	N	LYS	A	296	-0.038	-12.130	42.445	1.00	12.42
ATOM	1292	CA	LYS	A	296	-0.096	-13.576	42.572	1.00	10.90
ATOM	1293	CB	LYS	A	296	-0.924	-13.993	43.790	1.00	8.32
ATOM	1294	CG	LYS	A	296	-0.928	-15.496	44.071	1.00	5.48
ATOM	1295	CD	LYS	A	296	0.337	-15.957	44.762	1.00	3.51
ATOM	1296	CE	LYS	A	296	0.193	-17.388	45.229	1.00	7.63
ATOM	1297	NZ	LYS	A	296	1.418	-18.219	44.994	1.00	7.61
ATOM	1298	C	LYS	A	296	-0.663	-14.168	41.292	1.00	13.40
ATOM	1299	O	LYS	A	296	-1.756	-13.779	40.851	1.00	15.65
ATOM	1300	N	GLU	A	297	0.091	-15.088	40.690	1.00	13.26
ATOM	1301	CA	GLU	A	297	-0.369	-15.778	39.486	1.00	16.11
ATOM	1302	CB	GLU	A	297	0.771	-16.015	38.494	1.00	20.74
ATOM	1303	CG	GLU	A	297	1.824	-14.919	38.412	1.00	27.12
ATOM	1304	CD	GLU	A	297	3.235	-15.473	38.531	1.00	32.35
ATOM	1305	OE1	GLU	A	297	3.668	-16.234	37.625	1.00	35.73
ATOM	1306	OE2	GLU	A	297	3.910	-15.165	39.541	1.00	34.30
ATOM	1307	C	GLU	A	297	-1.040	-17.105	39.830	1.00	13.64
ATOM	1308	O	GLU	A	297	-1.010	-17.546	40.979	1.00	12.09
ATOM	1309	N	GLY	A	298	-1.659	-17.725	38.831	1.00	12.65
ATOM	1310	CA	GLY	A	298	-2.257	-19.041	38.994	1.00	17.89
ATOM	1311	C	GLY	A	298	-3.592	-19.077	39.715	1.00	20.28
ATOM	1312	O	GLY	A	298	-4.111	-20.154	40.006	1.00	19.05
ATOM	1313	N	ILE	A	299	-4.144	-17.900	39.993	1.00	25.39
ATOM	1314	CA	ILE	A	299	-5.447	-17.761	40.635	1.00	30.72
ATOM	1315	CB	ILE	A	299	-5.470	-16.472	41.517	1.00	33.04
ATOM	1316	CG1	ILE	A	299	-4.323	-16.460	42.547	1.00	34.26
ATOM	1317	CD1	ILE	A	299	-4.164	-17.736	43.394	1.00	36.04
ATOM	1318	CG2	ILE	A	299	-6.846	-16.261	42.177	1.00	34.45
ATOM	1319	C	ILE	A	299	-6.536	-17.684	39.571	1.00	32.52
ATOM	1320	O	ILE	A	299	-6.548	-16.754	38.767	1.00	31.64
ATOM	1321	N	SER	A	300	-7.450	-18.650	39.570	1.00	37.14
ATOM	1322	CA	SER	A	300	-8.537	-18.669	38.583	1.00	45.21
ATOM	1323	CB	SER	A	300	-8.220	-19.646	37.428	1.00	43.01
ATOM	1324	OG	SER	A	300	-8.321	-21.010	37.817	1.00	41.17
ATOM	1325	C	SER	A	300	-9.905	-18.973	39.219	1.00	51.19
ATOM	1326	O	SER	A	300	-9.996	-19.864	40.071	1.00	56.49
ATOM	1327	N	ASP	A	301	-10.945	-18.226	38.809	1.00	54.32
ATOM	1328	CA	ASP	A	301	-12.360	-18.433	39.227	1.00	56.18
ATOM	1329	CB	ASP	A	301	-12.817	-19.892	38.985	1.00	58.07
ATOM	1330	CG	ASP	A	301	-13.440	-20.100	37.610	1.00	59.00
ATOM	1331	OD1	ASP	A	301	-14.664	-20.350	37.550	1.00	58.53
ATOM	1332	OD2	ASP	A	301	-12.785	-20.046	36.542	1.00	58.87
ATOM	1333	C	ASP	A	301	-12.704	-17.987	40.671	1.00	55.93
ATOM	1334	O	ASP	A	301	-13.116	-16.845	40.902	1.00	56.42
ATOM	1335	N	GLY	A	302	-12.569	-18.912	41.621	1.00	55.03
ATOM	1336	CA	GLY	A	302	-12.685	-18.617	43.040	1.00	54.04
ATOM	1337	C	GLY	A	302	-11.393	-18.961	43.772	1.00	53.74
ATOM	1338	O	GLY	A	302	-10.863	-18.115	44.506	1.00	53.95
ATOM	1339	N	ALA	A	303	-10.897	-20.192	43.550	1.00	50.75
ATOM	1340	CA	ALA	A	303	-9.658	-20.733	44.153	1.00	45.71
ATOM	1341	CB	ALA	A	303	-8.966	-21.741	43.203	1.00	43.99

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1342	C	ALA	A	303	-8.679	-19.655	44.655	1.00	40.94
ATOM	1343	O	ALA	A	303	-8.212	-18.807	43.889	1.00	38.19
ATOM	1344	N	THR	A	304	-8.381	-19.727	45.954	1.00	36.35
ATOM	1345	CA	THR	A	304	-7.928	-18.585	46.748	1.00	29.90
ATOM	1346	CB	THR	A	304	-8.765	-18.488	48.033	1.00	29.06
ATOM	1347	OG1	THR	A	304	-8.877	-19.788	48.627	1.00	28.06
ATOM	1348	CG2	THR	A	304	-10.211	-18.077	47.727	1.00	29.14
ATOM	1349	C	THR	A	304	-6.455	-18.602	47.137	1.00	26.61
ATOM	1350	O	THR	A	304	-5.756	-19.589	46.919	1.00	27.47
ATOM	1351	N	MET	A	305	-6.022	-17.497	47.744	1.00	21.67
ATOM	1352	CA	MET	A	305	-4.636	-17.269	48.122	1.00	20.81
ATOM	1353	CB	MET	A	305	-4.018	-16.234	47.189	1.00	19.97
ATOM	1354	CG	MET	A	305	-4.730	-14.905	47.169	1.00	16.09
ATOM	1355	SD	MET	A	305	-4.325	-13.994	45.692	1.00	17.08
ATOM	1356	CE	MET	A	305	-5.913	-13.322	45.257	1.00	15.14
ATOM	1357	C	MET	A	305	-4.480	-16.820	49.585	1.00	22.96
ATOM	1358	O	MET	A	305	-5.350	-16.133	50.128	1.00	23.37
ATOM	1359	N	LYS	A	306	-3.338	-17.173	50.185	1.00	24.44
ATOM	1360	CA	LYS	A	306	-3.127	-17.144	51.643	1.00	22.17
ATOM	1361	CB	LYS	A	306	-2.407	-18.436	52.075	1.00	22.43
ATOM	1362	CG	LYS	A	306	-3.315	-19.566	52.582	1.00	23.73
ATOM	1363	CD	LYS	A	306	-2.582	-20.926	52.603	1.00	25.27
ATOM	1364	CE	LYS	A	306	-2.006	-21.281	53.986	1.00	23.74
ATOM	1365	NZ	LYS	A	306	-2.976	-22.017	54.847	1.00	22.13
ATOM	1366	C	LYS	A	306	-2.372	-15.934	52.241	1.00	20.52
ATOM	1367	O	LYS	A	306	-2.592	-15.594	53.402	1.00	23.31
ATOM	1368	N	TPO	A	307	-1.487	-15.303	51.471	1.00	15.84
ATOM	1369	CA	TPO	A	307	-0.529	-14.349	52.010	1.00	12.48
ATOM	1370	CB	TPO	A	307	0.428	-13.943	50.889	1.00	13.73
ATOM	1371	CG2	TPO	A	307	1.578	-13.043	51.340	1.00	13.62
ATOM	1372	OG1	TPO	A	307	0.965	-15.105	50.270	1.00	13.91
ATOM	1373	P	TPO	A	307	0.929	-15.315	48.673	1.00	10.79
ATOM	1374	O1P	TPO	A	307	2.301	-14.780	48.073	1.00	6.15
ATOM	1375	O3P	TPO	A	307	0.650	-16.863	48.393	1.00	7.66
ATOM	1376	O2P	TPO	A	307	-0.267	-14.495	48.033	1.00	14.09
ATOM	1377	C	TPO	A	307	-1.207	-13.102	52.470	1.00	14.73
ATOM	1378	O	TPO	A	307	-1.927	-12.479	51.700	1.00	17.22
ATOM	1379	N	PHE	A	308	-0.967	-12.719	53.723	1.00	14.16
ATOM	1380	CA	PHE	A	308	-1.412	-11.417	54.240	1.00	11.06
ATOM	1381	CB	PHE	A	308	-1.603	-11.481	55.767	1.00	9.57
ATOM	1382	CG	PHE	A	308	-1.814	-10.143	56.418	1.00	9.80
ATOM	1383	CD1	PHE	A	308	-0.840	-9.599	57.246	1.00	8.38
ATOM	1384	CE1	PHE	A	308	-1.039	-8.340	57.856	1.00	8.52
ATOM	1385	CZ	PHE	A	308	-2.227	-7.623	57.635	1.00	5.08
ATOM	1386	CE2	PHE	A	308	-3.207	-8.162	56.823	1.00	5.15
ATOM	1387	CD2	PHE	A	308	-3.000	-9.423	56.215	1.00	9.95
ATOM	1388	C	PHE	A	308	-0.385	-10.355	53.814	1.00	9.19
ATOM	1389	O	PHE	A	308	0.780	-10.412	54.213	1.00	8.70
ATOM	1390	N	CYS	A	309	-0.815	-9.411	52.977	1.00	8.03
ATOM	1391	CA	CYS	A	309	0.117	-8.506	52.286	1.00	6.30
ATOM	1392	CB	CYS	A	309	0.953	-9.303	51.294	1.00	5.84
ATOM	1393	SG	CYS	A	309	0.076	-9.585	49.739	1.00	6.28

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1394	C	CYS	A	309	-0.584	-7.396	51.508	1.00	4.40
ATOM	1395	O	CYS	A	309	-1.752	-7.541	51.107	1.00	4.55
ATOM	1396	N	GLY	A	310	0.130	-6.301	51.258	1.00	2.00
ATOM	1397	CA	GLY	A	310	-0.455	-5.220	50.478	1.00	3.38
ATOM	1398	C	GLY	A	310	-0.116	-3.855	51.003	1.00	4.67
ATOM	1399	O	GLY	A	310	1.047	-3.568	51.277	1.00	2.00
ATOM	1400	N	THR	A	311	-1.121	-2.997	51.137	1.00	8.60
ATOM	1401	CA	THR	A	311	-0.856	-1.690	51.733	1.00	14.76
ATOM	1402	CB	THR	A	311	-0.720	-0.594	50.676	1.00	16.15
ATOM	1403	OG1	THR	A	311	0.253	-1.001	49.709	1.00	22.33
ATOM	1404	CG2	THR	A	311	-0.064	0.624	51.275	1.00	15.85
ATOM	1405	C	THR	A	311	-1.863	-1.315	52.810	1.00	17.96
ATOM	1406	O	THR	A	311	-3.054	-1.168	52.522	1.00	20.47
ATOM	1407	N	PRO	A	312	-1.359	-1.153	54.042	1.00	18.77
ATOM	1408	CA	PRO	A	312	-2.187	-0.999	55.243	1.00	17.39
ATOM	1409	CB	PRO	A	312	-1.266	-0.236	56.200	1.00	21.08
ATOM	1410	CG	PRO	A	312	0.119	-0.139	55.502	1.00	19.52
ATOM	1411	CD	PRO	A	312	0.078	-1.093	54.374	1.00	19.18
ATOM	1412	C	PRO	A	312	-3.469	-0.215	55.009	1.00	17.23
ATOM	1413	O	PRO	A	312	-4.549	-0.694	55.343	1.00	21.66
ATOM	1414	N	GLU	A	313	-3.357	0.963	54.414	1.00	13.05
ATOM	1415	CA	GLU	A	313	-4.528	1.773	54.131	1.00	12.09
ATOM	1416	CB	GLU	A	313	-4.110	3.179	53.696	1.00	16.47
ATOM	1417	CG	GLU	A	313	-3.482	4.024	54.811	1.00	23.06
ATOM	1418	CD	GLU	A	313	-1.960	3.870	54.947	1.00	25.49
ATOM	1419	OE1	GLU	A	313	-1.369	2.922	54.356	1.00	26.10
ATOM	1420	OE2	GLU	A	313	-1.350	4.710	55.658	1.00	25.03
ATOM	1421	C	GLU	A	313	-5.460	1.154	53.096	1.00	9.65
ATOM	1422	O	GLU	A	313	-6.647	1.463	53.090	1.00	13.08
ATOM	1423	N	TYR	A	314	-4.939	0.285	52.234	1.00	6.62
ATOM	1424	CA	TYR	A	314	-5.689	-0.165	51.057	1.00	10.22
ATOM	1425	CB	TYR	A	314	-4.833	-0.064	49.796	1.00	10.80
ATOM	1426	CG	TYR	A	314	-4.593	1.328	49.275	1.00	11.28
ATOM	1427	CD1	TYR	A	314	-3.476	2.041	49.658	1.00	13.10
ATOM	1428	CE1	TYR	A	314	-3.239	3.317	49.177	1.00	15.53
ATOM	1429	CZ	TYR	A	314	-4.115	3.893	48.285	1.00	13.24
ATOM	1430	OH	TYR	A	314	-3.851	5.168	47.805	1.00	11.46
ATOM	1431	CE2	TYR	A	314	-5.227	3.189	47.880	1.00	12.73
ATOM	1432	CD2	TYR	A	314	-5.459	1.915	48.375	1.00	11.10
ATOM	1433	C	TYR	A	314	-6.181	-1.598	51.168	1.00	14.85
ATOM	1434	O	TYR	A	314	-6.773	-2.131	50.216	1.00	14.13
ATOM	1435	N	LEU	A	315	-5.927	-2.226	52.317	1.00	16.85
ATOM	1436	CA	LEU	A	315	-6.239	-3.645	52.505	1.00	16.59
ATOM	1437	CB	LEU	A	315	-5.567	-4.182	53.763	1.00	17.38
ATOM	1438	CG	LEU	A	315	-4.045	-4.146	53.817	1.00	18.06
ATOM	1439	CD1	LEU	A	315	-3.586	-4.489	55.218	1.00	18.85
ATOM	1440	CD2	LEU	A	315	-3.463	-5.101	52.804	1.00	18.81
ATOM	1441	C	LEU	A	315	-7.731	-3.946	52.566	1.00	17.42
ATOM	1442	O	LEU	A	315	-8.526	-3.155	53.091	1.00	20.19
ATOM	1443	N	ALA	A	316	-8.094	-5.103	52.025	1.00	17.44
ATOM	1444	CA	ALA	A	316	-9.475	-5.574	52.029	1.00	16.43
ATOM	1445	CB	ALA	A	316	-9.701	-6.541	50.879	1.00	17.27

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1446	C	ALA	A	316	-9.846	-6.235	53.353	1.00	14.45
ATOM	1447	O	ALA	A	316	-9.022	-6.938	53.962	1.00	11.13
ATOM	1448	N	PRO	A	317	-11.086	-6.005	53.797	1.00	13.89
ATOM	1449	CA	PRO	A	317	-11.632	-6.702	54.961	1.00	11.20
ATOM	1450	CB	PRO	A	317	-13.137	-6.511	54.786	1.00	5.63
ATOM	1451	CG	PRO	A	317	-13.250	-5.195	54.207	1.00	4.89
ATOM	1452	CD	PRO	A	317	-12.068	-5.047	53.254	1.00	10.86
ATOM	1453	C	PRO	A	317	-11.246	-8.185	55.000	1.00	12.09
ATOM	1454	O	PRO	A	317	-10.768	-8.621	56.041	1.00	15.68
ATOM	1455	N	GLU	A	318	-11.405	-8.930	53.908	1.00	10.93
ATOM	1456	CA	GLU	A	318	-11.122	-10.368	53.941	1.00	12.09
ATOM	1457	CB	GLU	A	318	-11.528	-11.089	52.642	1.00	14.71
ATOM	1458	CG	GLU	A	318	-10.907	-10.534	51.365	1.00	21.18
ATOM	1459	CD	GLU	A	318	-11.728	-9.434	50.694	1.00	24.13
ATOM	1460	OE1	GLU	A	318	-12.181	-8.487	51.384	1.00	24.60
ATOM	1461	OE2	GLU	A	318	-11.903	-9.503	49.456	1.00	25.49
ATOM	1462	C	GLU	A	318	-9.670	-10.627	54.301	1.00	11.22
ATOM	1463	O	GLU	A	318	-9.402	-11.409	55.199	1.00	15.25
ATOM	1464	N	VAL	A	319	-8.745	-9.941	53.636	1.00	9.45
ATOM	1465	CA	VAL	A	319	-7.324	-10.070	53.932	1.00	8.20
ATOM	1466	CB	VAL	A	319	-6.472	-9.065	53.117	1.00	7.43
ATOM	1467	CG1	VAL	A	319	-4.976	-9.411	53.172	1.00	4.93
ATOM	1468	CG2	VAL	A	319	-6.945	-9.013	51.672	1.00	9.50
ATOM	1469	C	VAL	A	319	-7.089	-9.857	55.424	1.00	10.41
ATOM	1470	O	VAL	A	319	-6.281	-10.563	56.035	1.00	9.70
ATOM	1471	N	LEU	A	320	-7.815	-8.899	56.005	1.00	12.04
ATOM	1472	CA	LEU	A	320	-7.639	-8.541	57.414	1.00	13.27
ATOM	1473	CB	LEU	A	320	-8.149	-7.126	57.706	1.00	7.97
ATOM	1474	CG	LEU	A	320	-7.085	-6.040	57.511	1.00	8.68
ATOM	1475	CD1	LEU	A	320	-7.639	-4.659	57.754	1.00	10.30
ATOM	1476	CD2	LEU	A	320	-5.876	-6.262	58.384	1.00	8.93
ATOM	1477	C	LEU	A	320	-8.234	-9.540	58.393	1.00	19.44
ATOM	1478	O	LEU	A	320	-7.848	-9.568	59.554	1.00	22.61
ATOM	1479	N	GLU	A	321	-9.177	-10.357	57.943	1.00	27.14
ATOM	1480	CA	GLU	A	321	-9.545	-11.538	58.706	1.00	34.83
ATOM	1481	CB	GLU	A	321	-10.963	-11.974	58.380	1.00	36.15
ATOM	1482	CG	GLU	A	321	-11.996	-11.232	59.200	1.00	42.19
ATOM	1483	CD	GLU	A	321	-13.255	-10.940	58.415	1.00	46.01
ATOM	1484	OE1	GLU	A	321	-14.349	-11.328	58.885	1.00	47.07
ATOM	1485	OE2	GLU	A	321	-13.150	-10.328	57.328	1.00	49.35
ATOM	1486	C	GLU	A	321	-8.541	-12.580	58.264	1.00	39.85
ATOM	1487	O	GLU	A	321	-7.323	-12.357	58.349	1.00	41.58
ATOM	1488	N	ASP	A	322	-9.033	-13.712	57.785	1.00	42.30
ATOM	1489	CA	ASP	A	322	-8.217	-14.531	56.913	1.00	45.72
ATOM	1490	CB	ASP	A	322	-7.074	-15.244	57.655	1.00	50.04
ATOM	1491	CG	ASP	A	322	-6.075	-15.907	56.695	1.00	55.00
ATOM	1492	OD1	ASP	A	322	-5.624	-15.225	55.738	1.00	57.17
ATOM	1493	OD2	ASP	A	322	-5.697	-17.101	56.813	1.00	54.91
ATOM	1494	C	ASP	A	322	-9.065	-15.517	56.161	1.00	46.88
ATOM	1495	O	ASP	A	322	-9.687	-15.168	55.143	1.00	45.15
ATOM	1496	N	ASN	A	323	-9.098	-16.737	56.703	1.00	47.64
ATOM	1497	CA	ASN	A	323	-9.403	-17.953	55.952	1.00	47.91

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1498	CB	ASN	A	323	-10.602	-18.704	56.552	1.00	49.15
ATOM	1499	CG	ASN	A	323	-10.180	-19.975	57.293	1.00	52.25
ATOM	1500	OD1	ASN	A	323	-9.600	-20.896	56.702	1.00	53.16
ATOM	1501	ND2	ASN	A	323	-10.467	-20.028	58.592	1.00	53.36
ATOM	1502	C	ASN	A	323	-9.494	-17.788	54.418	1.00	46.92
ATOM	1503	O	ASN	A	323	-10.518	-18.102	53.801	1.00	48.98
ATOM	1504	N	ASP	A	324	-8.415	-17.255	53.836	1.00	41.86
ATOM	1505	CA	ASP	A	324	-8.139	-17.358	52.408	1.00	37.08
ATOM	1506	CB	ASP	A	324	-8.090	-18.837	51.988	1.00	42.15
ATOM	1507	CG	ASP	A	324	-7.272	-19.700	52.964	1.00	46.60
ATOM	1508	OD1	ASP	A	324	-6.531	-19.120	53.795	1.00	49.52
ATOM	1509	OD2	ASP	A	324	-7.307	-20.955	52.986	1.00	48.00
ATOM	1510	C	ASP	A	324	-9.059	-16.534	51.507	1.00	32.79
ATOM	1511	O	ASP	A	324	-10.148	-16.969	51.132	1.00	32.67
ATOM	1512	N	TYR	A	325	-8.579	-15.347	51.154	1.00	28.14
ATOM	1513	CA	TYR	A	325	-9.261	-14.422	50.258	1.00	22.60
ATOM	1514	CB	TYR	A	325	-8.852	-12.992	50.599	1.00	24.02
ATOM	1515	CG	TYR	A	325	-7.376	-12.682	50.391	1.00	22.91
ATOM	1516	CD1	TYR	A	325	-6.910	-12.194	49.175	1.00	23.11
ATOM	1517	CE1	TYR	A	325	-5.578	-11.897	48.978	1.00	23.04
ATOM	1518	CZ	TYR	A	325	-4.684	-12.093	50.008	1.00	25.86
ATOM	1519	OH	TYR	A	325	-3.349	-11.802	49.816	1.00	29.42
ATOM	1520	CE2	TYR	A	325	-5.119	-12.577	51.230	1.00	24.57
ATOM	1521	CD2	TYR	A	325	-6.456	-12.862	51.417	1.00	23.79
ATOM	1522	C	TYR	A	325	-8.881	-14.687	48.819	1.00	20.02
ATOM	1523	O	TYR	A	325	-7.921	-15.399	48.558	1.00	18.90
ATOM	1524	N	GLY	A	326	-9.610	-14.070	47.889	1.00	21.15
ATOM	1525	CA	GLY	A	326	-9.350	-14.229	46.467	1.00	21.96
ATOM	1526	C	GLY	A	326	-9.438	-12.975	45.604	1.00	22.94
ATOM	1527	O	GLY	A	326	-9.273	-11.855	46.081	1.00	24.00
ATOM	1528	N	ARG	A	327	-9.723	-13.191	44.322	1.00	22.49
ATOM	1529	CA	ARG	A	327	-9.660	-12.188	43.253	1.00	18.40
ATOM	1530	CB	ARG	A	327	-10.276	-12.799	42.002	1.00	20.86
ATOM	1531	CG	ARG	A	327	-9.761	-12.273	40.692	1.00	22.09
ATOM	1532	CD	ARG	A	327	-10.362	-13.013	39.526	1.00	25.00
ATOM	1533	NE	ARG	A	327	-11.808	-13.124	39.691	1.00	27.42
ATOM	1534	CZ	ARG	A	327	-12.576	-13.948	38.999	1.00	30.21
ATOM	1535	NH1	ARG	A	327	-12.024	-14.742	38.095	1.00	33.39
ATOM	1536	NH2	ARG	A	327	-13.893	-13.985	39.204	1.00	29.71
ATOM	1537	C	ARG	A	327	-10.349	-10.856	43.516	1.00	16.87
ATOM	1538	O	ARG	A	327	-9.988	-9.844	42.918	1.00	17.74
ATOM	1539	N	ALA	A	328	-11.346	-10.858	44.395	1.00	15.65
ATOM	1540	CA	ALA	A	328	-12.162	-9.672	44.644	1.00	12.90
ATOM	1541	CB	ALA	A	328	-13.395	-10.052	45.411	1.00	12.66
ATOM	1542	C	ALA	A	328	-11.423	-8.546	45.366	1.00	14.00
ATOM	1543	O	ALA	A	328	-11.915	-7.425	45.430	1.00	17.90
ATOM	1544	N	VAL	A	329	-10.248	-8.837	45.910	1.00	14.94
ATOM	1545	CA	VAL	A	329	-9.480	-7.827	46.632	1.00	14.02
ATOM	1546	CB	VAL	A	329	-8.318	-8.436	47.445	1.00	9.86
ATOM	1547	CG1	VAL	A	329	-8.842	-9.487	48.371	1.00	10.74
ATOM	1548	CG2	VAL	A	329	-7.272	-9.022	46.554	1.00	6.17
ATOM	1549	C	VAL	A	329	-8.984	-6.703	45.720	1.00	17.59

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1550	O	VAL	A	329	-8.807	-5.564	46.170	1.00	18.03
ATOM	1551	N	ASP	A	330	-8.783	-7.006	44.440	1.00	20.06
ATOM	1552	CA	ASP	A	330	-8.391	-5.966	43.502	1.00	22.43
ATOM	1553	CB	ASP	A	330	-7.993	-6.555	42.156	1.00	24.76
ATOM	1554	CG	ASP	A	330	-6.584	-7.110	42.160	1.00	29.26
ATOM	1555	OD1	ASP	A	330	-5.930	-7.128	43.222	1.00	31.26
ATOM	1556	OD2	ASP	A	330	-6.039	-7.572	41.143	1.00	33.33
ATOM	1557	C	ASP	A	330	-9.524	-4.969	43.345	1.00	23.04
ATOM	1558	O	ASP	A	330	-9.292	-3.785	43.111	1.00	24.61
ATOM	1559	N	TRP	A	331	-10.756	-5.445	43.507	1.00	21.27
ATOM	1560	CA	TRP	A	331	-11.915	-4.572	43.336	1.00	16.46
ATOM	1561	CB	TRP	A	331	-13.129	-5.360	42.848	1.00	13.86
ATOM	1562	CG	TRP	A	331	-12.882	-6.126	41.553	1.00	12.21
ATOM	1563	CD1	TRP	A	331	-13.138	-7.445	41.336	1.00	15.09
ATOM	1564	NE1	TRP	A	331	-12.801	-7.799	40.050	1.00	15.16
ATOM	1565	CE2	TRP	A	331	-12.314	-6.700	39.398	1.00	12.76
ATOM	1566	CD2	TRP	A	331	-12.350	-5.621	40.312	1.00	11.92
ATOM	1567	CE3	TRP	A	331	-11.910	-4.369	39.874	1.00	13.68
ATOM	1568	CZ3	TRP	A	331	-11.454	-4.238	38.562	1.00	13.91
ATOM	1569	CH2	TRP	A	331	-11.421	-5.331	37.693	1.00	12.57
ATOM	1570	CZ2	TRP	A	331	-11.849	-6.567	38.088	1.00	11.93
ATOM	1571	C	TRP	A	331	-12.200	-3.693	44.563	1.00	12.65
ATOM	1572	O	TRP	A	331	-12.629	-2.546	44.429	1.00	9.35
ATOM	1573	N	TRP	A	332	-11.923	-4.213	45.751	1.00	11.41
ATOM	1574	CA	TRP	A	332	-11.787	-3.347	46.919	1.00	14.38
ATOM	1575	CB	TRP	A	332	-11.267	-4.130	48.110	1.00	12.68
ATOM	1576	CG	TRP	A	332	-11.080	-3.292	49.319	1.00	10.70
ATOM	1577	CD1	TRP	A	332	-9.926	-2.735	49.755	1.00	11.77
ATOM	1578	NE1	TRP	A	332	-10.142	-2.038	50.920	1.00	15.20
ATOM	1579	CE2	TRP	A	332	-11.467	-2.144	51.254	1.00	14.27
ATOM	1580	CD2	TRP	A	332	-12.086	-2.927	50.263	1.00	12.80
ATOM	1581	CE3	TRP	A	332	-13.461	-3.180	50.371	1.00	13.51
ATOM	1582	CZ3	TRP	A	332	-14.147	-2.664	51.440	1.00	13.25
ATOM	1583	CH2	TRP	A	332	-13.501	-1.887	52.413	1.00	12.67
ATOM	1584	CZ2	TRP	A	332	-12.168	-1.612	52.335	1.00	13.72
ATOM	1585	C	TRP	A	332	-10.791	-2.229	46.643	1.00	16.64
ATOM	1586	O	TRP	A	332	-11.116	-1.046	46.753	1.00	17.97
ATOM	1587	N	GLY	A	333	-9.567	-2.625	46.294	1.00	17.74
ATOM	1588	CA	GLY	A	333	-8.495	-1.684	46.064	1.00	15.88
ATOM	1589	C	GLY	A	333	-9.022	-0.588	45.174	1.00	17.44
ATOM	1590	O	GLY	A	333	-8.918	0.596	45.515	1.00	15.19
ATOM	1591	N	LEU	A	334	-9.629	-1.008	44.053	1.00	18.58
ATOM	1592	CA	LEU	A	334	-10.057	-0.108	42.983	1.00	16.11
ATOM	1593	CB	LEU	A	334	-10.790	-0.876	41.872	1.00	12.43
ATOM	1594	CG	LEU	A	334	-11.631	-0.033	40.901	1.00	11.62
ATOM	1595	CD1	LEU	A	334	-10.773	0.878	40.048	1.00	9.04
ATOM	1596	CD2	LEU	A	334	-12.507	-0.904	40.030	1.00	9.65
ATOM	1597	C	LEU	A	334	-10.935	0.960	43.589	1.00	16.13
ATOM	1598	O	LEU	A	334	-10.750	2.152	43.330	1.00	15.68
ATOM	1599	N	GLY	A	335	-11.847	0.493	44.439	1.00	13.78
ATOM	1600	CA	GLY	A	335	-12.798	1.323	45.142	1.00	13.31
ATOM	1601	C	GLY	A	335	-12.181	2.285	46.118	1.00	13.20

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1602	O	GLY	A	335	-12.675	3.394	46.246	1.00	19.17
ATOM	1603	N	VAL	A	336	-11.120	1.879	46.808	1.00	11.90
ATOM	1604	CA	VAL	A	336	-10.365	2.818	47.639	1.00	10.30
ATOM	1605	CB	VAL	A	336	-9.250	2.123	48.407	1.00	5.00
ATOM	1606	CG1	VAL	A	336	-8.512	3.107	49.260	1.00	2.00
ATOM	1607	CG2	VAL	A	336	-9.825	1.050	49.253	1.00	7.28
ATOM	1608	C	VAL	A	336	-9.771	3.926	46.757	1.00	13.19
ATOM	1609	O	VAL	A	336	-10.030	5.115	46.971	1.00	15.21
ATOM	1610	N	VAL	A	337	-9.000	3.516	45.754	1.00	13.29
ATOM	1611	CA	VAL	A	337	-8.400	4.429	44.782	1.00	13.05
ATOM	1612	CB	VAL	A	337	-7.611	3.619	43.731	1.00	11.85
ATOM	1613	CG1	VAL	A	337	-7.521	4.315	42.387	1.00	7.08
ATOM	1614	CG2	VAL	A	337	-6.229	3.330	44.277	1.00	14.96
ATOM	1615	C	VAL	A	337	-9.427	5.399	44.160	1.00	14.21
ATOM	1616	O	VAL	A	337	-9.225	6.617	44.141	1.00	12.98
ATOM	1617	N	MET	A	338	-10.545	4.863	43.695	1.00	13.70
ATOM	1618	CA	MET	A	338	-11.588	5.701	43.147	1.00	13.96
ATOM	1619	CB	MET	A	338	-12.711	4.847	42.611	1.00	17.57
ATOM	1620	CG	MET	A	338	-12.255	3.989	41.496	1.00	23.12
ATOM	1621	SD	MET	A	338	-12.444	4.883	40.013	1.00	26.77
ATOM	1622	CE	MET	A	338	-13.722	3.901	39.305	1.00	24.75
ATOM	1623	C	MET	A	338	-12.126	6.660	44.184	1.00	14.27
ATOM	1624	O	MET	A	338	-12.302	7.842	43.892	1.00	19.25
ATOM	1625	N	TYR	A	339	-12.378	6.160	45.391	1.00	10.05
ATOM	1626	CA	TYR	A	339	-12.918	6.990	46.466	1.00	9.15
ATOM	1627	CB	TYR	A	339	-13.059	6.152	47.732	1.00	7.31
ATOM	1628	CG	TYR	A	339	-13.783	6.840	48.864	1.00	7.19
ATOM	1629	CD1	TYR	A	339	-13.150	7.804	49.645	1.00	6.57
ATOM	1630	CE1	TYR	A	339	-13.813	8.426	50.685	1.00	6.77
ATOM	1631	CZ	TYR	A	339	-15.120	8.068	50.963	1.00	6.13
ATOM	1632	OH	TYR	A	339	-15.812	8.671	51.995	1.00	7.61
ATOM	1633	CE2	TYR	A	339	-15.747	7.104	50.211	1.00	4.44
ATOM	1634	CD2	TYR	A	339	-15.087	6.504	49.172	1.00	4.23
ATOM	1635	C	TYR	A	339	-11.968	8.159	46.727	1.00	9.95
ATOM	1636	O	TYR	A	339	-12.362	9.333	46.881	1.00	4.09
ATOM	1637	N	GLU	A	340	-10.695	7.808	46.763	1.00	8.87
ATOM	1638	CA	GLU	A	340	-9.678	8.770	47.021	1.00	8.82
ATOM	1639	CB	GLU	A	340	-8.339	8.092	47.060	1.00	13.95
ATOM	1640	CG	GLU	A	340	-7.805	7.904	48.455	1.00	17.74
ATOM	1641	CD	GLU	A	340	-6.506	7.144	48.427	1.00	23.24
ATOM	1642	OE1	GLU	A	340	-5.524	7.647	49.014	1.00	29.67
ATOM	1643	OE2	GLU	A	340	-6.464	6.060	47.802	1.00	22.69
ATOM	1644	C	GLU	A	340	-9.702	9.829	45.959	1.00	7.56
ATOM	1645	O	GLU	A	340	-9.693	10.992	46.311	1.00	14.77
ATOM	1646	N	MET	A	341	-9.756	9.441	44.681	1.00	3.16
ATOM	1647	CA	MET	A	341	-9.778	10.408	43.578	1.00	2.20
ATOM	1648	CB	MET	A	341	-9.800	9.715	42.233	1.00	2.13
ATOM	1649	CG	MET	A	341	-8.514	9.029	41.882	1.00	8.20
ATOM	1650	SD	MET	A	341	-8.502	8.404	40.209	1.00	15.10
ATOM	1651	CE	MET	A	341	-9.632	6.925	40.303	1.00	11.05
ATOM	1652	C	MET	A	341	-10.964	11.349	43.634	1.00	5.59
ATOM	1653	O	MET	A	341	-10.848	12.537	43.297	1.00	5.28

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1654	N	MET	A	342	-12.099	10.824	44.086	1.00	9.81
ATOM	1655	CA	MET	A	342	-13.366	11.541	44.002	1.00	9.64
ATOM	1656	CB	MET	A	342	-14.455	10.599	43.542	1.00	7.76
ATOM	1657	CG	MET	A	342	-14.436	10.382	42.073	1.00	6.50
ATOM	1658	SD	MET	A	342	-15.918	9.558	41.619	1.00	8.48
ATOM	1659	CE	MET	A	342	-15.483	7.811	42.026	1.00	10.33
ATOM	1660	C	MET	A	342	-13.821	12.247	45.259	1.00	11.25
ATOM	1661	O	MET	A	342	-14.480	13.274	45.169	1.00	14.95
ATOM	1662	N	CYS	A	343	-13.509	11.699	46.425	1.00	14.53
ATOM	1663	CA	CYS	A	343	-13.929	12.341	47.666	1.00	19.16
ATOM	1664	CB	CYS	A	343	-14.331	11.312	48.708	1.00	26.83
ATOM	1665	SG	CYS	A	343	-15.377	9.974	48.085	1.00	39.83
ATOM	1666	C	CYS	A	343	-12.826	13.208	48.221	1.00	17.73
ATOM	1667	O	CYS	A	343	-13.092	14.092	49.042	1.00	16.70
ATOM	1668	N	GLY	A	344	-11.600	12.936	47.759	1.00	15.57
ATOM	1669	CA	GLY	A	344	-10.393	13.618	48.200	1.00	13.42
ATOM	1670	C	GLY	A	344	-9.715	13.028	49.433	1.00	12.80
ATOM	1671	O	GLY	A	344	-8.841	13.654	50.028	1.00	14.05
ATOM	1672	N	ARG	A	345	-10.127	11.835	49.841	1.00	11.01
ATOM	1673	CA	ARG	A	345	-9.500	11.169	50.974	1.00	10.21
ATOM	1674	CB	ARG	A	345	-9.975	11.749	52.297	1.00	8.41
ATOM	1675	CG	ARG	A	345	-11.437	12.047	52.366	1.00	11.04
ATOM	1676	CD	ARG	A	345	-11.752	13.263	53.234	1.00	18.32
ATOM	1677	NE	ARG	A	345	-10.682	13.587	54.192	1.00	20.21
ATOM	1678	CZ	ARG	A	345	-10.214	14.820	54.437	1.00	21.73
ATOM	1679	NH1	ARG	A	345	-10.703	15.891	53.801	1.00	19.40
ATOM	1680	NH2	ARG	A	345	-9.239	14.979	55.325	1.00	22.31
ATOM	1681	C	ARG	A	345	-9.699	9.660	50.984	1.00	12.42
ATOM	1682	O	ARG	A	345	-10.582	9.118	50.315	1.00	16.50
ATOM	1683	N	LEU	A	346	-8.857	8.981	51.748	1.00	9.34
ATOM	1684	CA	LEU	A	346	-9.034	7.578	51.967	1.00	8.96
ATOM	1685	CB	LEU	A	346	-7.916	7.084	52.851	1.00	9.30
ATOM	1686	CG	LEU	A	346	-6.570	6.708	52.267	1.00	10.30
ATOM	1687	CD1	LEU	A	346	-5.658	6.426	53.448	1.00	13.78
ATOM	1688	CD2	LEU	A	346	-6.687	5.475	51.401	1.00	11.35
ATOM	1689	C	LEU	A	346	-10.368	7.401	52.688	1.00	13.73
ATOM	1690	O	LEU	A	346	-10.718	8.204	53.569	1.00	17.37
ATOM	1691	N	PRO	A	347	-11.107	6.351	52.346	1.00	12.75
ATOM	1692	CA	PRO	A	347	-12.399	6.097	52.980	1.00	11.53
ATOM	1693	CB	PRO	A	347	-12.947	4.929	52.172	1.00	11.57
ATOM	1694	CG	PRO	A	347	-11.732	4.222	51.711	1.00	14.66
ATOM	1695	CD	PRO	A	347	-10.751	5.301	51.381	1.00	13.94
ATOM	1696	C	PRO	A	347	-12.179	5.701	54.437	1.00	13.65
ATOM	1697	O	PRO	A	347	-13.024	5.956	55.297	1.00	17.03
ATOM	1698	N	PHE	A	348	-11.036	5.087	54.718	1.00	14.13
ATOM	1699	CA	PHE	A	348	-10.684	4.781	56.096	1.00	14.35
ATOM	1700	CB	PHE	A	348	-10.895	3.301	56.379	1.00	11.20
ATOM	1701	CG	PHE	A	348	-12.149	2.760	55.800	1.00	6.24
ATOM	1702	CD1	PHE	A	348	-13.318	2.791	56.525	1.00	2.00
ATOM	1703	CE1	PHE	A	348	-14.482	2.286	56.007	1.00	2.00
ATOM	1704	CZ	PHE	A	348	-14.493	1.757	54.734	1.00	5.53
ATOM	1705	CE2	PHE	A	348	-13.319	1.727	53.979	1.00	7.16

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1706	CD2	PHE	A	348	-12.158	2.223	54.519	1.00	6.89
ATOM	1707	C	PHE	A	348	-9.245	5.174	56.382	1.00	15.09
ATOM	1708	O	PHE	A	348	-8.346	4.818	55.624	1.00	15.00
ATOM	1709	N	TYR	A	349	-9.034	5.917	57.468	1.00	14.03
ATOM	1710	CA	TYR	A	349	-7.688	6.293	57.841	1.00	14.44
ATOM	1711	CB	TYR	A	349	-7.213	7.517	57.060	1.00	20.39
ATOM	1712	CG	TYR	A	349	-5.807	7.917	57.435	1.00	25.69
ATOM	1713	CD1	TYR	A	349	-4.712	7.255	56.892	1.00	26.63
ATOM	1714	CE1	TYR	A	349	-3.418	7.607	57.253	1.00	28.83
ATOM	1715	CZ	TYR	A	349	-3.211	8.622	58.171	1.00	28.13
ATOM	1716	OH	TYR	A	349	-1.925	8.967	58.517	1.00	31.56
ATOM	1717	CE2	TYR	A	349	-4.280	9.287	58.736	1.00	27.43
ATOM	1718	CD2	TYR	A	349	-5.573	8.929	58.370	1.00	27.30
ATOM	1719	C	TYR	A	349	-7.464	6.534	59.317	1.00	12.98
ATOM	1720	O	TYR	A	349	-8.288	7.122	60.007	1.00	16.82
ATOM	1721	N	ASN	A	350	-6.323	6.045	59.780	1.00	10.92
ATOM	1722	CA	ASN	A	350	-5.714	6.456	61.025	1.00	6.69
ATOM	1723	CB	ASN	A	350	-6.198	5.630	62.203	1.00	2.00
ATOM	1724	CG	ASN	A	350	-5.876	6.289	63.524	1.00	3.96
ATOM	1725	OD1	ASN	A	350	-5.679	5.626	64.533	1.00	6.29
ATOM	1726	ND2	ASN	A	350	-5.800	7.610	63.520	1.00	3.04
ATOM	1727	C	ASN	A	350	-4.220	6.317	60.861	1.00	8.60
ATOM	1728	O	ASN	A	350	-3.758	5.714	59.903	1.00	10.62
ATOM	1729	N	GLN	A	351	-3.452	6.903	61.765	1.00	11.60
ATOM	1730	CA	GLN	A	351	-2.011	6.718	61.720	1.00	14.45
ATOM	1731	CB	GLN	A	351	-1.268	7.922	62.317	1.00	13.31
ATOM	1732	CG	GLN	A	351	-1.726	8.365	63.698	1.00	12.80
ATOM	1733	CD	GLN	A	351	-2.971	9.231	63.681	1.00	11.44
ATOM	1734	OE1	GLN	A	351	-3.714	9.257	62.700	1.00	6.37
ATOM	1735	NE2	GLN	A	351	-3.206	9.938	64.782	1.00	13.56
ATOM	1736	C	GLN	A	351	-1.677	5.406	62.422	1.00	18.19
ATOM	1737	O	GLN	A	351	-0.907	4.595	61.903	1.00	19.31
ATOM	1738	N	ASP	A	352	-2.303	5.206	63.582	1.00	21.04
ATOM	1739	CA	ASP	A	352	-2.230	3.977	64.359	1.00	24.13
ATOM	1740	CB	ASP	A	352	-2.973	4.194	65.682	1.00	30.24
ATOM	1741	CG	ASP	A	352	-2.908	2.992	66.611	1.00	37.40
ATOM	1742	OD1	ASP	A	352	-3.359	1.901	66.196	1.00	41.72
ATOM	1743	OD2	ASP	A	352	-2.450	3.049	67.780	1.00	38.87
ATOM	1744	C	ASP	A	352	-2.831	2.814	63.556	1.00	24.61
ATOM	1745	O	ASP	A	352	-4.044	2.751	63.341	1.00	26.63
ATOM	1746	N	HIS	A	353	-1.968	1.903	63.110	1.00	23.40
ATOM	1747	CA	HIS	A	353	-2.355	0.819	62.208	1.00	20.40
ATOM	1748	CB	HIS	A	353	-1.134	-0.021	61.813	1.00	23.22
ATOM	1749	CG	HIS	A	353	-0.332	0.555	60.683	1.00	27.71
ATOM	1750	ND1	HIS	A	353	0.904	1.141	60.867	1.00	29.44
ATOM	1751	CE1	HIS	A	353	1.377	1.545	59.699	1.00	28.89
ATOM	1752	NE2	HIS	A	353	0.498	1.232	58.762	1.00	26.91
ATOM	1753	CD2	HIS	A	353	-0.581	0.615	59.351	1.00	27.75
ATOM	1754	C	HIS	A	353	-3.443	-0.077	62.789	1.00	17.83
ATOM	1755	O	HIS	A	353	-4.261	-0.594	62.039	1.00	17.31
ATOM	1756	N	GLU	A	354	-3.456	-0.257	64.113	1.00	18.43
ATOM	1757	CA	GLU	A	354	-4.460	-1.106	64.776	1.00	18.97

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1758	CB	GLU	A	354	-4.233	-1.226	66.293	1.00	22.59
ATOM	1759	CG	GLU	A	354	-2.918	-1.860	66.739	1.00	31.68
ATOM	1760	CD	GLU	A	354	-2.741	-1.848	68.266	1.00	38.26
ATOM	1761	OE1	GLU	A	354	-2.741	-0.745	68.875	1.00	38.41
ATOM	1762	OE2	GLU	A	354	-2.596	-2.945	68.869	1.00	40.21
ATOM	1763	C	GLU	A	354	-5.837	-0.518	64.534	1.00	15.95
ATOM	1764	O	GLU	A	354	-6.786	-1.249	64.254	1.00	15.29
ATOM	1765	N	LYS	A	355	-5.920	0.810	64.632	1.00	11.89
ATOM	1766	CA	LYS	A	355	-7.175	1.541	64.523	1.00	8.73
ATOM	1767	CB	LYS	A	355	-7.056	2.928	65.151	1.00	11.05
ATOM	1768	CG	LYS	A	355	-6.776	2.924	66.659	1.00	15.63
ATOM	1769	CD	LYS	A	355	-7.456	4.096	67.380	1.00	16.06
ATOM	1770	CE	LYS	A	355	-7.555	3.837	68.875	1.00	16.05
ATOM	1771	NZ	LYS	A	355	-7.529	2.378	69.172	1.00	13.84
ATOM	1772	C	LYS	A	355	-7.590	1.669	63.080	1.00	7.48
ATOM	1773	O	LYS	A	355	-8.771	1.653	62.766	1.00	8.66
ATOM	1774	N	LEU	A	356	-6.613	1.807	62.194	1.00	8.54
ATOM	1775	CA	LEU	A	356	-6.880	1.771	60.766	1.00	4.66
ATOM	1776	CB	LEU	A	356	-5.583	1.889	59.989	1.00	2.00
ATOM	1777	CG	LEU	A	356	-5.772	1.542	58.527	1.00	2.00
ATOM	1778	CD1	LEU	A	356	-6.488	2.715	57.863	1.00	2.00
ATOM	1779	CD2	LEU	A	356	-4.419	1.206	57.891	1.00	2.00
ATOM	1780	C	LEU	A	356	-7.619	0.477	60.406	1.00	6.08
ATOM	1781	O	LEU	A	356	-8.701	0.529	59.839	1.00	9.14
ATOM	1782	N	PHE	A	357	-7.048	-0.672	60.767	1.00	5.80
ATOM	1783	CA	PHE	A	357	-7.694	-1.969	60.564	1.00	6.03
ATOM	1784	CB	PHE	A	357	-6.784	-3.099	61.048	1.00	3.68
ATOM	1785	CG	PHE	A	357	-5.474	-3.206	60.303	1.00	3.15
ATOM	1786	CD1	PHE	A	357	-4.402	-3.893	60.865	1.00	4.03
ATOM	1787	CE1	PHE	A	357	-3.189	-4.004	60.193	1.00	2.00
ATOM	1788	CZ	PHE	A	357	-3.039	-3.431	58.952	1.00	2.00
ATOM	1789	CE2	PHE	A	357	-4.093	-2.751	58.378	1.00	2.00
ATOM	1790	CD2	PHE	A	357	-5.306	-2.641	59.049	1.00	2.68
ATOM	1791	C	PHE	A	357	-9.080	-2.078	61.235	1.00	9.65
ATOM	1792	O	PHE	A	357	-10.027	-2.571	60.632	1.00	10.22
ATOM	1793	N	GLU	A	358	-9.196	-1.623	62.480	1.00	15.70
ATOM	1794	CA	GLU	A	358	-10.487	-1.586	63.168	1.00	19.55
ATOM	1795	CB	GLU	A	358	-10.393	-0.751	64.457	1.00	24.82
ATOM	1796	CG	GLU	A	358	-11.227	-1.254	65.626	1.00	34.95
ATOM	1797	CD	GLU	A	358	-10.439	-1.360	66.942	1.00	43.24
ATOM	1798	OE1	GLU	A	358	-11.079	-1.444	68.022	1.00	45.63
ATOM	1799	OE2	GLU	A	358	-9.180	-1.371	66.918	1.00	45.90
ATOM	1800	C	GLU	A	358	-11.542	-1.003	62.222	1.00	18.14
ATOM	1801	O	GLU	A	358	-12.608	-1.592	62.038	1.00	19.53
ATOM	1802	N	LEU	A	359	-11.210	0.132	61.598	1.00	14.04
ATOM	1803	CA	LEU	A	359	-12.130	0.880	60.744	1.00	8.74
ATOM	1804	CB	LEU	A	359	-11.541	2.227	60.365	1.00	6.14
ATOM	1805	CG	LEU	A	359	-11.467	3.286	61.446	1.00	5.96
ATOM	1806	CD1	LEU	A	359	-10.567	4.398	60.965	1.00	5.93
ATOM	1807	CD2	LEU	A	359	-12.852	3.809	61.727	1.00	9.82
ATOM	1808	C	LEU	A	359	-12.475	0.139	59.476	1.00	9.26
ATOM	1809	O	LEU	A	359	-13.611	0.162	59.055	1.00	12.21

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1810	N	ILE	A	360	-11.493	-0.516	58.869	1.00	11.43
ATOM	1811	CA	ILE	A	360	-11.698	-1.250	57.620	1.00	10.30
ATOM	1812	CB	ILE	A	360	-10.347	-1.634	57.007	1.00	7.27
ATOM	1813	CG1	ILE	A	360	-9.638	-0.374	56.521	1.00	8.60
ATOM	1814	CD1	ILE	A	360	-8.114	-0.476	56.529	1.00	11.30
ATOM	1815	CG2	ILE	A	360	-10.526	-2.597	55.856	1.00	7.20
ATOM	1816	C	ILE	A	360	-12.623	-2.467	57.754	1.00	11.77
ATOM	1817	O	ILE	A	360	-13.270	-2.855	56.789	1.00	15.18
ATOM	1818	N	LEU	A	361	-12.699	-3.065	58.935	1.00	12.28
ATOM	1819	CA	LEU	A	361	-13.555	-4.229	59.108	1.00	15.34
ATOM	1820	CB	LEU	A	361	-12.917	-5.243	60.056	1.00	15.41
ATOM	1821	CG	LEU	A	361	-11.561	-5.857	59.742	1.00	15.18
ATOM	1822	CD1	LEU	A	361	-10.597	-5.492	60.845	1.00	13.37
ATOM	1823	CD2	LEU	A	361	-11.700	-7.367	59.621	1.00	15.77
ATOM	1824	C	LEU	A	361	-14.917	-3.861	59.665	1.00	19.43
ATOM	1825	O	LEU	A	361	-15.832	-4.679	59.630	1.00	23.44
ATOM	1826	N	MET	A	362	-15.059	-2.649	60.198	1.00	21.97
ATOM	1827	CA	MET	A	362	-16.203	-2.356	61.067	1.00	21.82
ATOM	1828	CB	MET	A	362	-15.799	-2.549	62.532	1.00	26.07
ATOM	1829	CG	MET	A	362	-15.409	-3.979	62.881	1.00	29.84
ATOM	1830	SD	MET	A	362	-15.264	-4.285	64.654	1.00	39.13
ATOM	1831	CE	MET	A	362	-14.784	-2.629	65.364	1.00	36.73
ATOM	1832	C	MET	A	362	-16.910	-1.009	60.897	1.00	17.65
ATOM	1833	O	MET	A	362	-18.030	-0.831	61.386	1.00	16.77
ATOM	1834	N	GLU	A	363	-16.266	-0.055	60.242	1.00	13.74
ATOM	1835	CA	GLU	A	363	-16.931	1.210	60.001	1.00	15.51
ATOM	1836	CB	GLU	A	363	-15.966	2.398	59.973	1.00	18.68
ATOM	1837	CG	GLU	A	363	-16.561	3.663	60.593	1.00	31.01
ATOM	1838	CD	GLU	A	363	-17.452	3.422	61.856	1.00	35.93
ATOM	1839	OE1	GLU	A	363	-16.941	3.569	63.002	1.00	33.27
ATOM	1840	OE2	GLU	A	363	-18.679	3.116	61.719	1.00	36.28
ATOM	1841	C	GLU	A	363	-17.708	1.115	58.722	1.00	14.52
ATOM	1842	O	GLU	A	363	-17.162	0.701	57.713	1.00	16.89
ATOM	1843	N	GLU	A	364	-18.992	1.469	58.779	1.00	15.11
ATOM	1844	CA	GLU	A	364	-19.842	1.498	57.597	1.00	13.83
ATOM	1845	CB	GLU	A	364	-21.301	1.639	57.994	1.00	19.07
ATOM	1846	CG	GLU	A	364	-22.261	1.741	56.819	1.00	27.20
ATOM	1847	CD	GLU	A	364	-23.493	0.882	57.022	1.00	35.18
ATOM	1848	OE1	GLU	A	364	-23.525	-0.246	56.461	1.00	38.36
ATOM	1849	OE2	GLU	A	364	-24.418	1.325	57.756	1.00	36.57
ATOM	1850	C	GLU	A	364	-19.427	2.684	56.744	1.00	9.11
ATOM	1851	O	GLU	A	364	-19.415	3.820	57.241	1.00	8.00
ATOM	1852	N	ILE	A	365	-19.087	2.399	55.480	1.00	2.46
ATOM	1853	CA	ILE	A	365	-18.591	3.383	54.519	1.00	2.00
ATOM	1854	CB	ILE	A	365	-18.508	2.771	53.104	1.00	2.00
ATOM	1855	CG1	ILE	A	365	-18.004	3.797	52.107	1.00	2.00
ATOM	1856	CD1	ILE	A	365	-16.534	3.631	51.825	1.00	7.55
ATOM	1857	CG2	ILE	A	365	-19.829	2.211	52.623	1.00	2.00
ATOM	1858	C	ILE	A	365	-19.394	4.678	54.488	1.00	6.75
ATOM	1859	O	ILE	A	365	-20.624	4.660	54.565	1.00	10.34
ATOM	1860	N	ARG	A	366	-18.708	5.810	54.381	1.00	8.02
ATOM	1861	CA	ARG	A	366	-19.431	7.071	54.286	1.00	7.06

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1862	CB	ARG	A	366	-19.236	7.880	55.555	1.00	8.35
ATOM	1863	CG	ARG	A	366	-19.736	7.175	56.794	1.00	12.15
ATOM	1864	CD	ARG	A	366	-19.268	7.803	58.083	1.00	15.18
ATOM	1865	NE	ARG	A	366	-17.854	8.135	57.999	1.00	16.46
ATOM	1866	CZ	ARG	A	366	-17.181	8.835	58.895	1.00	16.58
ATOM	1867	NH1	ARG	A	366	-17.781	9.308	59.978	1.00	14.84
ATOM	1868	NH2	ARG	A	366	-15.891	9.064	58.699	1.00	18.16
ATOM	1869	C	ARG	A	366	-19.029	7.868	53.046	1.00	7.11
ATOM	1870	O	ARG	A	366	-17.892	7.755	52.579	1.00	8.22
ATOM	1871	N	PHE	A	367	-19.964	8.656	52.511	1.00	2.00
ATOM	1872	CA	PHE	A	367	-19.679	9.482	51.348	1.00	2.00
ATOM	1873	CB	PHE	A	367	-20.386	8.974	50.107	1.00	2.00
ATOM	1874	CG	PHE	A	367	-20.239	7.526	49.902	1.00	2.00
ATOM	1875	CD1	PHE	A	367	-19.098	7.025	49.351	1.00	2.00
ATOM	1876	CE1	PHE	A	367	-18.945	5.682	49.180	1.00	6.88
ATOM	1877	CZ	PHE	A	367	-19.962	4.826	49.551	1.00	8.38
ATOM	1878	CE2	PHE	A	367	-21.117	5.330	50.095	1.00	3.01
ATOM	1879	CD2	PHE	A	367	-21.246	6.662	50.270	1.00	2.00
ATOM	1880	C	PHE	A	367	-20.068	10.914	51.575	1.00	2.00
ATOM	1881	O	PHE	A	367	-21.084	11.177	52.202	1.00	2.00
ATOM	1882	N	PRO	A	368	-19.215	11.818	51.073	1.00	4.91
ATOM	1883	CA	PRO	A	368	-19.438	13.259	51.105	1.00	2.00
ATOM	1884	CB	PRO	A	368	-18.320	13.797	50.230	1.00	2.29
ATOM	1885	CG	PRO	A	368	-17.240	12.835	50.409	1.00	6.63
ATOM	1886	CD	PRO	A	368	-17.917	11.495	50.445	1.00	7.01
ATOM	1887	C	PRO	A	368	-20.729	13.579	50.443	1.00	2.99
ATOM	1888	O	PRO	A	368	-20.998	13.116	49.325	1.00	2.00
ATOM	1889	N	ARG	A	369	-21.509	14.396	51.141	1.00	5.03
ATOM	1890	CA	ARG	A	369	-22.850	14.733	50.739	1.00	3.72
ATOM	1891	CB	ARG	A	369	-23.365	15.888	51.579	1.00	7.65
ATOM	1892	CG	ARG	A	369	-24.719	15.626	52.204	1.00	9.47
ATOM	1893	CD	ARG	A	369	-25.829	15.484	51.201	1.00	9.66
ATOM	1894	NE	ARG	A	369	-26.866	16.473	51.426	1.00	9.67
ATOM	1895	CZ	ARG	A	369	-28.026	16.187	51.978	1.00	10.71
ATOM	1896	NH1	ARG	A	369	-28.276	14.934	52.347	1.00	11.69
ATOM	1897	NH2	ARG	A	369	-28.934	17.143	52.163	1.00	10.99
ATOM	1898	C	ARG	A	369	-22.873	15.091	49.280	1.00	6.32
ATOM	1899	O	ARG	A	369	-23.819	14.757	48.595	1.00	10.60
ATOM	1900	N	THR	A	370	-21.809	15.743	48.813	1.00	9.67
ATOM	1901	CA	THR	A	370	-21.677	16.193	47.423	1.00	9.89
ATOM	1902	CB	THR	A	370	-20.444	17.099	47.254	1.00	12.56
ATOM	1903	OG1	THR	A	370	-19.264	16.420	47.730	1.00	12.80
ATOM	1904	CG2	THR	A	370	-20.580	18.342	48.147	1.00	12.18
ATOM	1905	C	THR	A	370	-21.642	15.055	46.418	1.00	6.63
ATOM	1906	O	THR	A	370	-22.650	14.763	45.821	1.00	12.38
ATOM	1907	N	LEU	A	371	-20.494	14.423	46.235	1.00	6.19
ATOM	1908	CA	LEU	A	371	-20.316	13.310	45.285	1.00	10.00
ATOM	1909	CB	LEU	A	371	-19.373	12.274	45.890	1.00	9.60
ATOM	1910	CG	LEU	A	371	-19.355	10.867	45.314	1.00	5.30
ATOM	1911	CD1	LEU	A	371	-17.944	10.607	44.839	1.00	5.99
ATOM	1912	CD2	LEU	A	371	-19.795	9.859	46.361	1.00	3.04
ATOM	1913	C	LEU	A	371	-21.587	12.606	44.819	1.00	10.68

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1914	O	LEU	A	371	-22.356	12.131	45.648	1.00	14.90
ATOM	1915	N	GLY	A	372	-21.755	12.495	43.496	1.00	12.62
ATOM	1916	CA	GLY	A	372	-22.994	12.057	42.854	1.00	14.23
ATOM	1917	C	GLY	A	372	-23.426	10.584	42.918	1.00	17.99
ATOM	1918	O	GLY	A	372	-22.618	9.682	43.214	1.00	13.97
ATOM	1919	N	PRO	A	373	-24.706	10.347	42.593	1.00	18.71
ATOM	1920	CA	PRO	A	373	-25.390	9.062	42.820	1.00	19.50
ATOM	1921	CB	PRO	A	373	-26.781	9.319	42.242	1.00	16.42
ATOM	1922	CG	PRO	A	373	-26.583	10.417	41.270	1.00	14.30
ATOM	1923	CD	PRO	A	373	-25.606	11.314	41.940	1.00	17.57
ATOM	1924	C	PRO	A	373	-24.752	7.833	42.143	1.00	21.10
ATOM	1925	O	PRO	A	373	-24.542	6.826	42.820	1.00	20.43
ATOM	1926	N	GLU	A	374	-24.485	7.917	40.839	1.00	22.94
ATOM	1927	CA	GLU	A	374	-23.759	6.884	40.108	1.00	23.93
ATOM	1928	CB	GLU	A	374	-23.542	7.282	38.636	1.00	29.70
ATOM	1929	CG	GLU	A	374	-23.741	8.774	38.304	1.00	41.13
ATOM	1930	CD	GLU	A	374	-22.653	9.710	38.883	1.00	47.03
ATOM	1931	OE1	GLU	A	374	-21.468	9.659	38.436	1.00	48.15
ATOM	1932	OE2	GLU	A	374	-22.986	10.519	39.789	1.00	46.39
ATOM	1933	C	GLU	A	374	-22.430	6.548	40.816	1.00	23.18
ATOM	1934	O	GLU	A	374	-22.226	5.403	41.210	1.00	27.76
ATOM	1935	N	ALA	A	375	-21.549	7.534	41.014	1.00	19.13
ATOM	1936	CA	ALA	A	375	-20.269	7.314	41.719	1.00	15.51
ATOM	1937	CB	ALA	A	375	-19.458	8.576	41.731	1.00	16.49
ATOM	1938	C	ALA	A	375	-20.432	6.797	43.148	1.00	13.68
ATOM	1939	O	ALA	A	375	-19.704	5.902	43.583	1.00	7.47
ATOM	1940	N	LYS	A	376	-21.401	7.375	43.866	1.00	15.49
ATOM	1941	CA	LYS	A	376	-21.757	6.928	45.213	1.00	13.73
ATOM	1942	CB	LYS	A	376	-22.922	7.737	45.786	1.00	10.52
ATOM	1943	CG	LYS	A	376	-22.830	7.940	47.288	1.00	10.89
ATOM	1944	CD	LYS	A	376	-24.037	8.668	47.842	1.00	14.93
ATOM	1945	CE	LYS	A	376	-23.665	9.986	48.489	1.00	16.52
ATOM	1946	NZ	LYS	A	376	-24.387	11.112	47.840	1.00	19.42
ATOM	1947	C	LYS	A	376	-22.094	5.455	45.214	1.00	13.09
ATOM	1948	O	LYS	A	376	-21.755	4.752	46.154	1.00	14.09
ATOM	1949	N	SER	A	377	-22.743	5.004	44.141	1.00	14.13
ATOM	1950	CA	SER	A	377	-23.130	3.607	43.950	1.00	15.25
ATOM	1951	CB	SER	A	377	-24.243	3.511	42.894	1.00	14.83
ATOM	1952	OG	SER	A	377	-24.388	2.201	42.373	1.00	16.34
ATOM	1953	C	SER	A	377	-21.943	2.708	43.577	1.00	16.37
ATOM	1954	O	SER	A	377	-21.725	1.657	44.198	1.00	14.21
ATOM	1955	N	LEU	A	378	-21.178	3.116	42.567	1.00	16.17
ATOM	1956	CA	LEU	A	378	-20.029	2.326	42.160	1.00	17.04
ATOM	1957	CB	LEU	A	378	-19.255	2.989	41.025	1.00	14.67
ATOM	1958	CG	LEU	A	378	-17.890	2.364	40.736	1.00	11.76
ATOM	1959	CD1	LEU	A	378	-18.033	1.024	40.038	1.00	11.34
ATOM	1960	CD2	LEU	A	378	-17.072	3.292	39.901	1.00	12.30
ATOM	1961	C	LEU	A	378	-19.119	2.079	43.351	1.00	17.65
ATOM	1962	O	LEU	A	378	-18.641	0.954	43.542	1.00	18.82
ATOM	1963	N	LEU	A	379	-18.917	3.126	44.153	1.00	14.53
ATOM	1964	CA	LEU	A	379	-18.048	3.051	45.320	1.00	14.73
ATOM	1965	CB	LEU	A	379	-17.826	4.434	45.916	1.00	16.09

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	1966	CG	LEU	A	379	-16.878	5.318	45.098	1.00	20.41
ATOM	1967	CD1	LEU	A	379	-16.374	6.478	45.938	1.00	21.62
ATOM	1968	CD2	LEU	A	379	-15.706	4.530	44.482	1.00	19.01
ATOM	1969	C	LEU	A	379	-18.612	2.111	46.357	1.00	13.13
ATOM	1970	O	LEU	A	379	-18.013	1.083	46.669	1.00	12.02
ATOM	1971	N	SER	A	380	-19.786	2.467	46.860	1.00	14.58
ATOM	1972	CA	SER	A	380	-20.576	1.617	47.741	1.00	14.20
ATOM	1973	CB	SER	A	380	-22.035	2.076	47.758	1.00	8.63
ATOM	1974	OG	SER	A	380	-22.568	1.963	49.063	1.00	8.09
ATOM	1975	C	SER	A	380	-20.512	0.156	47.329	1.00	16.32
ATOM	1976	O	SER	A	380	-20.367	-0.713	48.190	1.00	18.70
ATOM	1977	N	GLY	A	381	-20.613	-0.096	46.018	1.00	16.95
ATOM	1978	CA	GLY	A	381	-20.575	-1.437	45.458	1.00	15.44
ATOM	1979	C	GLY	A	381	-19.194	-2.036	45.586	1.00	18.09
ATOM	1980	O	GLY	A	381	-19.023	-3.159	46.077	1.00	21.76
ATOM	1981	N	LEU	A	382	-18.192	-1.265	45.178	1.00	16.17
ATOM	1982	CA	LEU	A	382	-16.829	-1.757	45.177	1.00	8.34
ATOM	1983	CB	LEU	A	382	-15.913	-0.816	44.416	1.00	3.25
ATOM	1984	CG	LEU	A	382	-16.022	-0.733	42.890	1.00	3.54
ATOM	1985	CD1	LEU	A	382	-15.416	0.566	42.395	1.00	3.71
ATOM	1986	CD2	LEU	A	382	-15.353	-1.916	42.220	1.00	2.00
ATOM	1987	C	LEU	A	382	-16.326	-1.901	46.575	1.00	10.35
ATOM	1988	O	LEU	A	382	-15.334	-2.563	46.788	1.00	19.95
ATOM	1989	N	LEU	A	383	-16.981	-1.277	47.542	1.00	11.20
ATOM	1990	CA	LEU	A	383	-16.438	-1.292	48.906	1.00	13.21
ATOM	1991	CB	LEU	A	383	-16.120	0.129	49.416	1.00	8.87
ATOM	1992	CG	LEU	A	383	-14.894	0.790	48.798	1.00	6.84
ATOM	1993	CD1	LEU	A	383	-15.057	2.269	48.787	1.00	7.23
ATOM	1994	CD2	LEU	A	383	-13.639	0.417	49.544	1.00	11.95
ATOM	1995	C	LEU	A	383	-17.287	-2.081	49.910	1.00	15.85
ATOM	1996	O	LEU	A	383	-17.208	-1.863	51.128	1.00	16.68
ATOM	1997	N	LYS	A	384	-18.087	-3.013	49.404	1.00	15.31
ATOM	1998	CA	LYS	A	384	-18.679	-4.008	50.281	1.00	14.09
ATOM	1999	CB	LYS	A	384	-19.651	-4.879	49.502	1.00	12.53
ATOM	2000	CG	LYS	A	384	-21.080	-4.475	49.721	1.00	14.38
ATOM	2001	CD	LYS	A	384	-21.640	-3.759	48.507	1.00	17.18
ATOM	2002	CE	LYS	A	384	-23.140	-4.038	48.328	1.00	18.85
ATOM	2003	NZ	LYS	A	384	-23.973	-3.410	49.387	1.00	19.04
ATOM	2004	C	LYS	A	384	-17.574	-4.840	50.982	1.00	13.85
ATOM	2005	O	LYS	A	384	-16.525	-5.158	50.390	1.00	13.11
ATOM	2006	N	LYS	A	385	-17.802	-5.150	52.253	1.00	11.59
ATOM	2007	CA	LYS	A	385	-16.804	-5.826	53.068	1.00	12.04
ATOM	2008	CB	LYS	A	385	-17.063	-5.581	54.545	1.00	9.30
ATOM	2009	CG	LYS	A	385	-17.188	-4.138	54.885	1.00	7.03
ATOM	2010	CD	LYS	A	385	-16.208	-3.764	55.946	1.00	5.61
ATOM	2011	CE	LYS	A	385	-16.613	-2.461	56.584	1.00	6.56
ATOM	2012	NZ	LYS	A	385	-15.998	-1.321	55.843	1.00	9.18
ATOM	2013	C	LYS	A	385	-16.749	-7.318	52.793	1.00	17.00
ATOM	2014	O	LYS	A	385	-15.660	-7.897	52.731	1.00	19.47
ATOM	2015	N	ASP	A	386	-17.910	-7.955	52.652	1.00	20.71
ATOM	2016	CA	ASP	A	386	-17.920	-9.340	52.208	1.00	25.16
ATOM	2017	CB	ASP	A	386	-19.183	-10.083	52.624	1.00	29.20

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2018	CG	ASP	A	386	-19.322	-11.411	51.895	1.00	33.93
ATOM	2019	OD1	ASP	A	386	-19.802	-11.386	50.742	1.00	34.87
ATOM	2020	OD2	ASP	A	386	-18.939	-12.513	52.366	1.00	36.62
ATOM	2021	C	ASP	A	386	-17.742	-9.406	50.689	1.00	25.90
ATOM	2022	O	ASP	A	386	-18.517	-8.803	49.943	1.00	26.86
ATOM	2023	N	PRO	A	387	-16.742	-10.162	50.236	1.00	25.68
ATOM	2024	CA	PRO	A	387	-16.328	-10.140	48.832	1.00	24.61
ATOM	2025	CB	PRO	A	387	-15.070	-10.995	48.831	1.00	25.30
ATOM	2026	CG	PRO	A	387	-14.684	-11.112	50.264	1.00	26.40
ATOM	2027	CD	PRO	A	387	-15.949	-11.118	51.028	1.00	26.16
ATOM	2028	C	PRO	A	387	-17.370	-10.770	47.928	1.00	26.24
ATOM	2029	O	PRO	A	387	-17.449	-10.407	46.750	1.00	29.56
ATOM	2030	N	LYS	A	388	-18.170	-11.685	48.475	1.00	23.34
ATOM	2031	CA	LYS	A	388	-19.192	-12.370	47.687	1.00	20.87
ATOM	2032	CB	LYS	A	388	-19.858	-13.498	48.488	1.00	20.71
ATOM	2033	CG	LYS	A	388	-18.910	-14.284	49.395	1.00	22.88
ATOM	2034	CD	LYS	A	388	-19.416	-15.682	49.674	1.00	25.38
ATOM	2035	CE	LYS	A	388	-18.912	-16.664	48.623	1.00	29.08
ATOM	2036	NZ	LYS	A	388	-19.845	-17.822	48.432	1.00	32.58
ATOM	2037	C	LYS	A	388	-20.228	-11.376	47.157	1.00	18.56
ATOM	2038	O	LYS	A	388	-20.881	-11.635	46.146	1.00	21.02
ATOM	2039	N	GLN	A	389	-20.347	-10.233	47.832	1.00	14.34
ATOM	2040	CA	GLN	A	389	-21.299	-9.191	47.450	1.00	10.32
ATOM	2041	CB	GLN	A	389	-22.126	-8.760	48.647	1.00	6.71
ATOM	2042	CG	GLN	A	389	-22.820	-9.868	49.349	1.00	8.49
ATOM	2043	CD	GLN	A	389	-24.087	-9.400	49.982	1.00	13.62
ATOM	2044	OE1	GLN	A	389	-24.245	-8.207	50.273	1.00	17.67
ATOM	2045	NE2	GLN	A	389	-25.014	-10.323	50.191	1.00	16.98
ATOM	2046	C	GLN	A	389	-20.606	-7.968	46.869	1.00	9.84
ATOM	2047	O	GLN	A	389	-21.260	-6.979	46.550	1.00	9.03
ATOM	2048	N	ARG	A	390	-19.288	-8.023	46.738	1.00	8.38
ATOM	2049	CA	ARG	A	390	-18.570	-6.907	46.157	1.00	10.59
ATOM	2050	CB	ARG	A	390	-17.084	-7.002	46.462	1.00	12.48
ATOM	2051	CG	ARG	A	390	-16.373	-5.667	46.362	1.00	14.11
ATOM	2052	CD	ARG	A	390	-14.951	-5.667	46.908	1.00	13.49
ATOM	2053	NE	ARG	A	390	-14.894	-6.129	48.282	1.00	12.63
ATOM	2054	CZ	ARG	A	390	-14.009	-7.009	48.726	1.00	16.63
ATOM	2055	NH1	ARG	A	390	-13.083	-7.512	47.905	1.00	13.48
ATOM	2056	NH2	ARG	A	390	-14.041	-7.378	50.002	1.00	17.94
ATOM	2057	C	ARG	A	390	-18.780	-6.866	44.659	1.00	12.58
ATOM	2058	O	ARG	A	390	-18.759	-7.899	43.994	1.00	16.45
ATOM	2059	N	LEU	A	391	-18.989	-5.669	44.132	1.00	14.13
ATOM	2060	CA	LEU	A	391	-19.121	-5.480	42.695	1.00	15.13
ATOM	2061	CB	LEU	A	391	-19.425	-4.008	42.386	1.00	15.53
ATOM	2062	CG	LEU	A	391	-19.725	-3.569	40.953	1.00	17.60
ATOM	2063	CD1	LEU	A	391	-21.190	-3.692	40.671	1.00	20.74
ATOM	2064	CD2	LEU	A	391	-19.305	-2.130	40.762	1.00	20.61
ATOM	2065	C	LEU	A	391	-17.843	-5.970	41.998	1.00	15.47
ATOM	2066	O	LEU	A	391	-16.769	-5.392	42.155	1.00	14.75
ATOM	2067	N	GLY	A	392	-17.967	-7.066	41.262	1.00	15.12
ATOM	2068	CA	GLY	A	392	-16.828	-7.660	40.587	1.00	17.84
ATOM	2069	C	GLY	A	392	-16.357	-8.910	41.303	1.00	20.98

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2070	O	GLY	A	392	-15.473	-9.630	40.818	1.00	22.43
ATOM	2071	N	GLY	A	393	-16.959	-9.167	42.463	1.00	20.09
ATOM	2072	CA	GLY	A	393	-16.612	-10.312	43.283	1.00	16.71
ATOM	2073	C	GLY	A	393	-17.370	-11.560	42.908	1.00	14.93
ATOM	2074	O	GLY	A	393	-17.251	-12.571	43.594	1.00	12.93
ATOM	2075	N	GLY	A	394	-18.143	-11.473	41.824	1.00	16.03
ATOM	2076	CA	GLY	A	394	-18.918	-12.584	41.301	1.00	17.57
ATOM	2077	C	GLY	A	394	-18.175	-13.308	40.196	1.00	19.56
ATOM	2078	O	GLY	A	394	-17.091	-12.888	39.788	1.00	18.92
ATOM	2079	N	SER	A	395	-18.758	-14.400	39.704	1.00	24.04
ATOM	2080	CA	SER	A	395	-18.100	-15.238	38.692	1.00	25.88
ATOM	2081	CB	SER	A	395	-18.886	-16.531	38.449	1.00	23.26
ATOM	2082	OG	SER	A	395	-19.769	-16.385	37.356	1.00	20.98
ATOM	2083	C	SER	A	395	-17.892	-14.471	37.389	1.00	26.74
ATOM	2084	O	SER	A	395	-17.107	-14.869	36.534	1.00	29.07
ATOM	2085	N	GLU	A	396	-18.602	-13.360	37.263	1.00	28.31
ATOM	2086	CA	GLU	A	396	-18.481	-12.484	36.109	1.00	28.63
ATOM	2087	CB	GLU	A	396	-19.735	-11.603	35.983	1.00	32.93
ATOM	2088	CG	GLU	A	396	-20.983	-12.323	35.479	1.00	33.78
ATOM	2089	CD	GLU	A	396	-20.770	-13.049	34.157	1.00	35.89
ATOM	2090	OE1	GLU	A	396	-19.819	-12.700	33.417	1.00	36.68
ATOM	2091	OE2	GLU	A	396	-21.560	-13.974	33.852	1.00	36.45
ATOM	2092	C	GLU	A	396	-17.215	-11.623	36.154	1.00	24.68
ATOM	2093	O	GLU	A	396	-16.606	-11.364	35.126	1.00	24.78
ATOM	2094	N	ASP	A	397	-16.835	-11.177	37.345	1.00	22.19
ATOM	2095	CA	ASP	A	397	-15.623	-10.382	37.543	1.00	20.91
ATOM	2096	CB	ASP	A	397	-14.378	-11.115	37.003	1.00	19.88
ATOM	2097	CG	ASP	A	397	-13.075	-10.575	37.582	1.00	19.17
ATOM	2098	OD1	ASP	A	397	-12.996	-10.330	38.805	1.00	18.63
ATOM	2099	OD2	ASP	A	397	-12.073	-10.355	36.879	1.00	19.50
ATOM	2100	C	ASP	A	397	-15.738	-8.955	36.990	1.00	20.29
ATOM	2101	O	ASP	A	397	-16.717	-8.263	37.251	1.00	21.60
ATOM	2102	N	ALA	A	398	-14.730	-8.527	36.235	1.00	17.86
ATOM	2103	CA	ALA	A	398	-14.608	-7.157	35.758	1.00	13.23
ATOM	2104	CB	ALA	A	398	-13.297	-6.997	35.003	1.00	12.08
ATOM	2105	C	ALA	A	398	-15.781	-6.692	34.886	1.00	15.62
ATOM	2106	O	ALA	A	398	-16.081	-5.496	34.835	1.00	14.95
ATOM	2107	N	LYS	A	399	-16.432	-7.626	34.189	1.00	16.02
ATOM	2108	CA	LYS	A	399	-17.551	-7.273	33.334	1.00	13.91
ATOM	2109	CB	LYS	A	399	-18.051	-8.479	32.547	1.00	17.50
ATOM	2110	CG	LYS	A	399	-19.096	-8.158	31.458	1.00	25.65
ATOM	2111	CD	LYS	A	399	-18.517	-7.314	30.303	1.00	29.81
ATOM	2112	CE	LYS	A	399	-19.613	-6.624	29.472	1.00	31.23
ATOM	2113	NZ	LYS	A	399	-19.138	-5.328	28.890	1.00	30.95
ATOM	2114	C	LYS	A	399	-18.657	-6.633	34.181	1.00	13.96
ATOM	2115	O	LYS	A	399	-19.251	-5.638	33.775	1.00	17.10
ATOM	2116	N	GLU	A	400	-18.890	-7.175	35.372	1.00	11.25
ATOM	2117	CA	GLU	A	400	-19.871	-6.629	36.308	1.00	10.44
ATOM	2118	CB	GLU	A	400	-19.843	-7.433	37.609	1.00	15.28
ATOM	2119	CG	GLU	A	400	-20.876	-7.011	38.644	1.00	21.17
ATOM	2120	CD	GLU	A	400	-21.075	-8.047	39.740	1.00	24.54
ATOM	2121	OE1	GLU	A	400	-20.243	-9.001	39.849	1.00	24.52

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2122	OE2	GLU	A	400	-22.075	-7.894	40.489	1.00	24.68
ATOM	2123	C	GLU	A	400	-19.675	-5.130	36.588	1.00	7.48
ATOM	2124	O	GLU	A	400	-20.627	-4.350	36.521	1.00	8.69
ATOM	2125	N	ILE	A	401	-18.439	-4.749	36.898	1.00	4.25
ATOM	2126	CA	ILE	A	401	-18.050	-3.364	37.112	1.00	2.00
ATOM	2127	CB	ILE	A	401	-16.592	-3.292	37.537	1.00	2.00
ATOM	2128	CG1	ILE	A	401	-16.424	-3.713	38.982	1.00	2.00
ATOM	2129	CD1	ILE	A	401	-14.981	-3.785	39.366	1.00	2.00
ATOM	2130	CG2	ILE	A	401	-16.035	-1.900	37.324	1.00	2.00
ATOM	2131	C	ILE	A	401	-18.181	-2.562	35.837	1.00	3.17
ATOM	2132	O	ILE	A	401	-18.612	-1.412	35.870	1.00	8.59
ATOM	2133	N	MET	A	402	-17.775	-3.146	34.716	1.00	2.00
ATOM	2134	CA	MET	A	402	-17.805	-2.418	33.457	1.00	5.25
ATOM	2135	CB	MET	A	402	-17.162	-3.219	32.340	1.00	8.13
ATOM	2136	CG	MET	A	402	-15.688	-3.489	32.519	1.00	12.00
ATOM	2137	SD	MET	A	402	-15.070	-4.549	31.204	1.00	13.70
ATOM	2138	CE	MET	A	402	-13.342	-4.323	31.370	1.00	18.16
ATOM	2139	C	MET	A	402	-19.224	-2.056	33.065	1.00	7.97
ATOM	2140	O	MET	A	402	-19.457	-0.980	32.524	1.00	12.30
ATOM	2141	N	GLN	A	403	-20.181	-2.936	33.340	1.00	10.04
ATOM	2142	CA	GLN	A	403	-21.560	-2.632	32.984	1.00	14.71
ATOM	2143	CB	GLN	A	403	-22.295	-3.868	32.436	1.00	17.30
ATOM	2144	CG	GLN	A	403	-22.528	-5.003	33.437	1.00	21.10
ATOM	2145	CD	GLN	A	403	-22.767	-6.365	32.777	1.00	21.02
ATOM	2146	OE1	GLN	A	403	-22.443	-6.568	31.600	1.00	21.82
ATOM	2147	NE2	GLN	A	403	-23.321	-7.301	33.544	1.00	20.17
ATOM	2148	C	GLN	A	403	-22.332	-1.897	34.092	1.00	16.89
ATOM	2149	O	GLN	A	403	-23.555	-1.809	34.048	1.00	19.63
ATOM	2150	N	HIS	A	404	-21.608	-1.346	35.066	1.00	20.40
ATOM	2151	CA	HIS	A	404	-22.199	-0.470	36.086	1.00	20.49
ATOM	2152	CB	HIS	A	404	-21.240	-0.253	37.258	1.00	19.20
ATOM	2153	CG	HIS	A	404	-21.867	0.439	38.434	1.00	23.38
ATOM	2154	ND1	HIS	A	404	-22.411	1.706	38.355	1.00	22.39
ATOM	2155	CE1	HIS	A	404	-22.873	2.060	39.541	1.00	22.77
ATOM	2156	NE2	HIS	A	404	-22.650	1.071	40.389	1.00	24.02
ATOM	2157	CD2	HIS	A	404	-22.024	0.043	39.722	1.00	24.27
ATOM	2158	C	HIS	A	404	-22.582	0.870	35.478	1.00	19.31
ATOM	2159	O	HIS	A	404	-21.863	1.379	34.609	1.00	18.03
ATOM	2160	N	ARG	A	405	-23.705	1.431	35.948	1.00	20.12
ATOM	2161	CA	ARG	A	405	-24.279	2.667	35.380	1.00	19.49
ATOM	2162	CB	ARG	A	405	-25.522	3.208	36.154	1.00	26.30
ATOM	2163	CG	ARG	A	405	-26.203	2.287	37.226	1.00	34.75
ATOM	2164	CD	ARG	A	405	-26.704	3.019	38.529	1.00	40.05
ATOM	2165	NE	ARG	A	405	-27.325	2.125	39.534	1.00	45.09
ATOM	2166	CZ	ARG	A	405	-27.555	2.427	40.831	1.00	46.58
ATOM	2167	NH1	ARG	A	405	-27.225	3.614	41.335	1.00	47.07
ATOM	2168	NH2	ARG	A	405	-28.139	1.536	41.631	1.00	45.92
ATOM	2169	C	ARG	A	405	-23.203	3.741	35.252	1.00	13.15
ATOM	2170	O	ARG	A	405	-23.203	4.510	34.296	1.00	7.53
ATOM	2171	N	PHE	A	406	-22.274	3.751	36.206	1.00	8.31
ATOM	2172	CA	PHE	A	406	-21.176	4.711	36.247	1.00	8.69
ATOM	2173	CB	PHE	A	406	-20.263	4.375	37.411	1.00	7.28

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2174	CG	PHE	A	406	-19.132	5.342	37.614	1.00	8.21
ATOM	2175	CD1	PHE	A	406	-19.304	6.486	38.397	1.00	7.87
ATOM	2176	CE1	PHE	A	406	-18.250	7.368	38.631	1.00	6.30
ATOM	2177	CZ	PHE	A	406	-17.013	7.130	38.086	1.00	4.86
ATOM	2178	CE2	PHE	A	406	-16.822	5.992	37.301	1.00	11.39
ATOM	2179	CD2	PHE	A	406	-17.880	5.090	37.077	1.00	7.66
ATOM	2180	C	PHE	A	406	-20.359	4.782	34.957	1.00	10.86
ATOM	2181	O	PHE	A	406	-20.048	5.878	34.487	1.00	15.89
ATOM	2182	N	PHE	A	407	-19.997	3.629	34.401	1.00	9.05
ATOM	2183	CA	PHE	A	407	-19.290	3.592	33.126	1.00	10.03
ATOM	2184	CB	PHE	A	407	-18.272	2.455	33.100	1.00	9.81
ATOM	2185	CG	PHE	A	407	-17.283	2.492	34.218	1.00	11.46
ATOM	2186	CD1	PHE	A	407	-17.313	1.523	35.214	1.00	12.13
ATOM	2187	CE1	PHE	A	407	-16.390	1.552	36.260	1.00	12.46
ATOM	2188	CZ	PHE	A	407	-15.409	2.548	36.300	1.00	10.97
ATOM	2189	CE2	PHE	A	407	-15.359	3.508	35.310	1.00	9.95
ATOM	2190	CD2	PHE	A	407	-16.297	3.480	34.271	1.00	12.99
ATOM	2191	C	PHE	A	407	-20.321	3.449	31.993	1.00	13.09
ATOM	2192	O	PHE	A	407	-20.269	2.527	31.146	1.00	13.19
ATOM	2193	N	ALA	A	408	-21.262	4.384	31.988	1.00	12.26
ATOM	2194	CA	ALA	A	408	-22.454	4.246	31.178	1.00	13.45
ATOM	2195	CB	ALA	A	408	-23.487	5.232	31.613	1.00	17.35
ATOM	2196	C	ALA	A	408	-22.171	4.400	29.703	1.00	12.66
ATOM	2197	O	ALA	A	408	-22.472	3.510	28.914	1.00	13.17
ATOM	2198	N	GLY	A	409	-21.596	5.534	29.332	1.00	12.46
ATOM	2199	CA	GLY	A	409	-21.367	5.820	27.932	1.00	15.37
ATOM	2200	C	GLY	A	409	-20.243	5.002	27.346	1.00	15.57
ATOM	2201	O	GLY	A	409	-20.086	4.931	26.122	1.00	18.02
ATOM	2202	N	ILE	A	410	-19.498	4.356	28.240	1.00	14.24
ATOM	2203	CA	ILE	A	410	-18.184	3.798	27.952	1.00	10.40
ATOM	2204	CB	ILE	A	410	-17.421	3.577	29.293	1.00	8.70
ATOM	2205	CG1	ILE	A	410	-17.453	4.838	30.163	1.00	8.11
ATOM	2206	CD1	ILE	A	410	-17.234	6.165	29.419	1.00	10.58
ATOM	2207	CG2	ILE	A	410	-15.992	3.152	29.054	1.00	7.34
ATOM	2208	C	ILE	A	410	-18.268	2.509	27.149	1.00	8.15
ATOM	2209	O	ILE	A	410	-18.843	1.523	27.617	1.00	7.91
ATOM	2210	N	VAL	A	411	-17.701	2.541	25.942	1.00	5.79
ATOM	2211	CA	VAL	A	411	-17.562	1.365	25.081	1.00	7.84
ATOM	2212	CB	VAL	A	411	-17.639	1.771	23.594	1.00	6.79
ATOM	2213	CG1	VAL	A	411	-16.876	0.792	22.704	1.00	5.60
ATOM	2214	CG2	VAL	A	411	-19.088	1.904	23.154	1.00	7.51
ATOM	2215	C	VAL	A	411	-16.190	0.774	25.376	1.00	10.04
ATOM	2216	O	VAL	A	411	-15.176	1.431	25.146	1.00	14.94
ATOM	2217	N	TRP	A	412	-16.132	-0.449	25.887	1.00	8.39
ATOM	2218	CA	TRP	A	412	-14.870	-0.906	26.468	1.00	7.36
ATOM	2219	CB	TRP	A	412	-15.102	-2.010	27.489	1.00	7.46
ATOM	2220	CG	TRP	A	412	-15.767	-1.441	28.681	1.00	6.78
ATOM	2221	CD1	TRP	A	412	-17.106	-1.290	28.878	1.00	6.79
ATOM	2222	NE1	TRP	A	412	-17.344	-0.688	30.089	1.00	4.22
ATOM	2223	CE2	TRP	A	412	-16.147	-0.422	30.691	1.00	5.59
ATOM	2224	CD2	TRP	A	412	-15.130	-0.878	29.821	1.00	5.75
ATOM	2225	CE3	TRP	A	412	-13.796	-0.721	30.208	1.00	4.31

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2226	CZ3	TRP	A	412	-13.523	-0.130	31.428	1.00	6.57
ATOM	2227	CH2	TRP	A	412	-14.562	0.316	32.273	1.00	7.77
ATOM	2228	CZ2	TRP	A	412	-15.876	0.175	31.921	1.00	6.37
ATOM	2229	C	TRP	A	412	-13.779	-1.253	25.472	1.00	7.76
ATOM	2230	O	TRP	A	412	-12.604	-1.069	25.760	1.00	5.78
ATOM	2231	N	GLN	A	413	-14.179	-1.711	24.289	1.00	12.61
ATOM	2232	CA	GLN	A	413	-13.245	-1.960	23.192	1.00	13.87
ATOM	2233	CB	GLN	A	413	-14.018	-2.428	21.948	1.00	15.66
ATOM	2234	CG	GLN	A	413	-13.170	-3.026	20.811	1.00	19.47
ATOM	2235	CD	GLN	A	413	-12.166	-4.066	21.293	1.00	21.00
ATOM	2236	OE1	GLN	A	413	-12.549	-5.179	21.656	1.00	22.65
ATOM	2237	NE2	GLN	A	413	-10.882	-3.708	21.292	1.00	19.40
ATOM	2238	C	GLN	A	413	-12.418	-0.698	22.903	1.00	14.24
ATOM	2239	O	GLN	A	413	-11.291	-0.776	22.411	1.00	11.50
ATOM	2240	N	HIS	A	414	-12.991	0.455	23.248	1.00	16.94
ATOM	2241	CA	HIS	A	414	-12.385	1.766	23.022	1.00	17.62
ATOM	2242	CB	HIS	A	414	-13.468	2.848	23.006	1.00	19.87
ATOM	2243	CG	HIS	A	414	-14.076	3.082	21.663	1.00	20.19
ATOM	2244	ND1	HIS	A	414	-13.908	2.215	20.604	1.00	20.96
ATOM	2245	CE1	HIS	A	414	-14.552	2.681	19.551	1.00	21.64
ATOM	2246	NE2	HIS	A	414	-15.132	3.820	19.888	1.00	22.51
ATOM	2247	CD2	HIS	A	414	-14.849	4.093	21.205	1.00	20.49
ATOM	2248	C	HIS	A	414	-11.349	2.119	24.084	1.00	16.49
ATOM	2249	O	HIS	A	414	-10.235	2.546	23.749	1.00	17.52
ATOM	2250	N	VAL	A	415	-11.729	1.960	25.355	1.00	12.06
ATOM	2251	CA	VAL	A	415	-10.839	2.235	26.479	1.00	10.57
ATOM	2252	CB	VAL	A	415	-11.373	1.604	27.781	1.00	11.67
ATOM	2253	CG1	VAL	A	415	-10.326	1.615	28.882	1.00	12.86
ATOM	2254	CG2	VAL	A	415	-12.597	2.324	28.246	1.00	13.26
ATOM	2255	C	VAL	A	415	-9.486	1.645	26.156	1.00	10.82
ATOM	2256	O	VAL	A	415	-8.478	2.346	26.185	1.00	10.89
ATOM	2257	N	TYR	A	416	-9.505	0.357	25.813	1.00	11.93
ATOM	2258	CA	TYR	A	416	-8.336	-0.425	25.444	1.00	14.80
ATOM	2259	CB	TYR	A	416	-8.768	-1.857	25.112	1.00	17.60
ATOM	2260	CG	TYR	A	416	-7.634	-2.783	24.736	1.00	20.78
ATOM	2261	CD1	TYR	A	416	-6.969	-3.524	25.712	1.00	22.95
ATOM	2262	CE1	TYR	A	416	-5.927	-4.369	25.381	1.00	27.08
ATOM	2263	CZ	TYR	A	416	-5.535	-4.484	24.053	1.00	29.57
ATOM	2264	OH	TYR	A	416	-4.497	-5.330	23.726	1.00	34.35
ATOM	2265	CE2	TYR	A	416	-6.181	-3.758	23.058	1.00	25.68
ATOM	2266	CD2	TYR	A	416	-7.224	-2.917	23.406	1.00	21.99
ATOM	2267	C	TYR	A	416	-7.576	0.161	24.262	1.00	16.68
ATOM	2268	O	TYR	A	416	-6.349	0.264	24.284	1.00	16.33
ATOM	2269	N	GLU	A	417	-8.303	0.541	23.222	1.00	20.09
ATOM	2270	CA	GLU	A	417	-7.653	1.034	22.024	1.00	24.16
ATOM	2271	CB	GLU	A	417	-8.603	0.959	20.823	1.00	28.25
ATOM	2272	CG	GLU	A	417	-8.317	-0.235	19.916	1.00	34.46
ATOM	2273	CD	GLU	A	417	-9.559	-0.843	19.265	1.00	38.53
ATOM	2274	OE1	GLU	A	417	-10.606	-0.153	19.176	1.00	41.35
ATOM	2275	OE2	GLU	A	417	-9.479	-2.018	18.823	1.00	38.88
ATOM	2276	C	GLU	A	417	-7.064	2.433	22.220	1.00	24.63
ATOM	2277	O	GLU	A	417	-6.575	3.030	21.263	1.00	27.05

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2278	N	LYS	A	418	-7.085	2.926	23.463	1.00	24.74
ATOM	2279	CA	LYS	A	418	-6.534	4.239	23.839	1.00	24.89
ATOM	2280	CB	LYS	A	418	-5.022	4.324	23.550	1.00	27.02
ATOM	2281	CG	LYS	A	418	-4.111	3.705	24.604	1.00	29.36
ATOM	2282	CD	LYS	A	418	-2.970	4.658	25.001	1.00	31.86
ATOM	2283	CE	LYS	A	418	-1.603	3.970	25.020	1.00	32.41
ATOM	2284	NZ	LYS	A	418	-0.820	4.259	23.782	1.00	34.20
ATOM	2285	C	LYS	A	418	-7.275	5.360	23.110	1.00	23.86
ATOM	2286	O	LYS	A	418	-6.665	6.246	22.500	1.00	23.82
ATOM	2287	N	LYS	A	419	-8.598	5.313	23.162	1.00	21.27
ATOM	2288	CA	LYS	A	419	-9.382	6.235	22.365	1.00	20.30
ATOM	2289	CB	LYS	A	419	-10.243	5.491	21.335	1.00	21.32
ATOM	2290	CG	LYS	A	419	-9.764	5.665	19.889	1.00	22.89
ATOM	2291	CD	LYS	A	419	-9.481	4.318	19.199	1.00	24.64
ATOM	2292	CE	LYS	A	419	-9.389	4.457	17.670	1.00	26.40
ATOM	2293	NZ	LYS	A	419	-9.932	3.266	16.942	1.00	26.48
ATOM	2294	C	LYS	A	419	-10.212	7.159	23.225	1.00	19.91
ATOM	2295	O	LYS	A	419	-10.781	8.119	22.715	1.00	24.88
ATOM	2296	N	LEU	A	420	-10.287	6.879	24.522	1.00	17.22
ATOM	2297	CA	LEU	A	420	-10.801	7.860	25.468	1.00	16.76
ATOM	2298	CB	LEU	A	420	-10.765	7.300	26.882	1.00	16.60
ATOM	2299	CG	LEU	A	420	-12.082	6.922	27.553	1.00	17.80
ATOM	2300	CD1	LEU	A	420	-11.811	5.953	28.688	1.00	18.43
ATOM	2301	CD2	LEU	A	420	-12.811	8.152	28.074	1.00	20.69
ATOM	2302	C	LEU	A	420	-9.874	9.066	25.384	1.00	17.86
ATOM	2303	O	LEU	A	420	-8.698	8.910	25.049	1.00	19.46
ATOM	2304	N	SER	A	421	-10.380	10.264	25.652	1.00	17.80
ATOM	2305	CA	SER	A	421	-9.490	11.423	25.671	1.00	19.78
ATOM	2306	CB	SER	A	421	-10.115	12.642	25.001	1.00	21.15
ATOM	2307	OG	SER	A	421	-9.183	13.712	24.998	1.00	22.32
ATOM	2308	C	SER	A	421	-9.052	11.759	27.091	1.00	17.99
ATOM	2309	O	SER	A	421	-9.904	11.967	27.958	1.00	21.61
ATOM	2310	N	PRO	A	422	-7.733	11.828	27.316	1.00	14.82
ATOM	2311	CA	PRO	A	422	-7.161	11.975	28.667	1.00	12.99
ATOM	2312	CB	PRO	A	422	-5.661	11.729	28.451	1.00	11.78
ATOM	2313	CG	PRO	A	422	-5.559	11.175	27.066	1.00	12.55
ATOM	2314	CD	PRO	A	422	-6.679	11.793	26.290	1.00	14.08
ATOM	2315	C	PRO	A	422	-7.388	13.364	29.243	1.00	10.04
ATOM	2316	O	PRO	A	422	-7.011	14.357	28.622	1.00	13.43
ATOM	2317	N	PRO	A	423	-7.998	13.420	30.419	1.00	5.22
ATOM	2318	CA	PRO	A	423	-8.457	14.673	31.026	1.00	3.86
ATOM	2319	CB	PRO	A	423	-9.195	14.190	32.255	1.00	5.07
ATOM	2320	CG	PRO	A	423	-8.527	12.914	32.578	1.00	5.83
ATOM	2321	CD	PRO	A	423	-8.292	12.256	31.261	1.00	3.68
ATOM	2322	C	PRO	A	423	-7.323	15.605	31.442	1.00	6.00
ATOM	2323	O	PRO	A	423	-7.570	16.813	31.541	1.00	5.41
ATOM	2324	N	PHE	A	424	-6.128	15.057	31.692	1.00	6.47
ATOM	2325	CA	PHE	A	424	-4.916	15.864	31.898	1.00	6.25
ATOM	2326	CB	PHE	A	424	-4.600	16.013	33.388	1.00	4.23
ATOM	2327	CG	PHE	A	424	-3.158	16.291	33.670	1.00	3.18
ATOM	2328	CD1	PHE	A	424	-2.670	17.588	33.635	1.00	2.66
ATOM	2329	CE1	PHE	A	424	-1.324	17.860	33.875	1.00	2.00

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2330	CZ	PHE	A	424	-0.460	16.831	34.144	1.00	2.52
ATOM	2331	CE2	PHE	A	424	-0.935	15.510	34.176	1.00	5.37
ATOM	2332	CD2	PHE	A	424	-2.277	15.252	33.945	1.00	4.69
ATOM	2333	C	PHE	A	424	-3.689	15.311	31.153	1.00	8.77
ATOM	2334	O	PHE	A	424	-3.235	14.198	31.448	1.00	11.40
ATOM	2335	N	LYS	A	425	-3.150	16.093	30.207	1.00	10.06
ATOM	2336	CA	LYS	A	425	-1.941	15.708	29.461	1.00	12.05
ATOM	2337	CB	LYS	A	425	-2.044	16.089	27.975	1.00	13.73
ATOM	2338	CG	LYS	A	425	-0.799	15.726	27.126	1.00	17.23
ATOM	2339	CD	LYS	A	425	-0.807	16.424	25.744	1.00	19.83
ATOM	2340	CE	LYS	A	425	0.395	16.019	24.861	1.00	19.75
ATOM	2341	NZ	LYS	A	425	0.140	14.829	23.972	1.00	15.66
ATOM	2342	C	LYS	A	425	-0.688	16.328	30.077	1.00	12.47
ATOM	2343	O	LYS	A	425	-0.617	17.548	30.216	1.00	12.89
ATOM	2344	N	PRO	A	426	0.293	15.498	30.445	1.00	13.17
ATOM	2345	CA	PRO	A	426	1.544	15.985	31.032	1.00	12.94
ATOM	2346	CB	PRO	A	426	2.363	14.709	31.235	1.00	11.47
ATOM	2347	CG	PRO	A	426	1.390	13.649	31.300	1.00	13.23
ATOM	2348	CD	PRO	A	426	0.291	14.030	30.336	1.00	14.38
ATOM	2349	C	PRO	A	426	2.270	16.928	30.085	1.00	15.53
ATOM	2350	O	PRO	A	426	2.402	16.673	28.877	1.00	15.98
ATOM	2351	N	GLN	A	427	2.731	18.031	30.655	1.00	17.00
ATOM	2352	CA	GLN	A	427	3.370	19.077	29.888	1.00	19.77
ATOM	2353	CB	GLN	A	427	2.754	20.437	30.255	1.00	21.17
ATOM	2354	CG	GLN	A	427	1.258	20.538	29.937	1.00	21.21
ATOM	2355	CD	GLN	A	427	1.001	20.967	28.507	1.00	21.46
ATOM	2356	OE1	GLN	A	427	1.154	22.144	28.188	1.00	25.85
ATOM	2357	NE2	GLN	A	427	0.627	20.022	27.641	1.00	17.80
ATOM	2358	C	GLN	A	427	4.855	19.026	30.182	1.00	18.92
ATOM	2359	O	GLN	A	427	5.305	19.557	31.192	1.00	18.67
ATOM	2360	N	VAL	A	428	5.612	18.374	29.305	1.00	20.29
ATOM	2361	CA	VAL	A	428	7.032	18.124	29.573	1.00	22.77
ATOM	2362	CB	VAL	A	428	7.332	16.607	29.687	1.00	22.73
ATOM	2363	CG1	VAL	A	428	7.250	16.164	31.129	1.00	21.19
ATOM	2364	CG2	VAL	A	428	6.375	15.788	28.810	1.00	25.01
ATOM	2365	C	VAL	A	428	7.998	18.768	28.569	1.00	22.85
ATOM	2366	O	VAL	A	428	7.976	18.424	27.385	1.00	22.93
ATOM	2367	N	THR	A	429	8.841	19.688	29.054	1.00	21.94
ATOM	2368	CA	THR	A	429	9.901	20.294	28.239	1.00	22.99
ATOM	2369	CB	THR	A	429	10.802	21.281	29.057	1.00	22.41
ATOM	2370	OG1	THR	A	429	10.960	20.820	30.401	1.00	21.36
ATOM	2371	CG2	THR	A	429	10.129	22.630	29.230	1.00	24.23
ATOM	2372	C	THR	A	429	10.767	19.230	27.560	1.00	23.72
ATOM	2373	O	THR	A	429	10.651	19.010	26.354	1.00	24.52
ATOM	2374	N	SER	A	430	11.618	18.570	28.342	1.00	24.66
ATOM	2375	CA	SER	A	430	12.521	17.542	27.827	1.00	26.61
ATOM	2376	CB	SER	A	430	13.908	17.648	28.493	1.00	27.85
ATOM	2377	OG	SER	A	430	13.836	18.114	29.835	1.00	27.62
ATOM	2378	C	SER	A	430	11.936	16.131	27.982	1.00	26.95
ATOM	2379	O	SER	A	430	10.785	15.972	28.386	1.00	29.17
ATOM	2380	N	GLU	A	431	12.722	15.118	27.625	1.00	27.55
ATOM	2381	CA	GLU	A	431	12.372	13.727	27.896	1.00	28.48

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2382	CB	GLU	A	431	12.876	12.808	26.772	1.00	34.87
ATOM	2383	CG	GLU	A	431	11.797	12.315	25.807	1.00	41.73
ATOM	2384	CD	GLU	A	431	10.501	11.912	26.507	1.00	46.70
ATOM	2385	OE1	GLU	A	431	10.511	10.885	27.250	1.00	46.51
ATOM	2386	OE2	GLU	A	431	9.480	12.634	26.314	1.00	47.10
ATOM	2387	C	GLU	A	431	12.974	13.315	29.238	1.00	24.07
ATOM	2388	O	GLU	A	431	12.554	12.339	29.855	1.00	22.58
ATOM	2389	N	THR	A	432	13.968	14.081	29.669	1.00	20.65
ATOM	2390	CA	THR	A	432	14.663	13.861	30.924	1.00	17.87
ATOM	2391	CB	THR	A	432	16.121	14.357	30.805	1.00	18.34
ATOM	2392	OG1	THR	A	432	16.836	14.016	31.993	1.00	19.58
ATOM	2393	CG2	THR	A	432	16.198	15.892	30.794	1.00	18.90
ATOM	2394	C	THR	A	432	13.958	14.597	32.046	1.00	17.44
ATOM	2395	O	THR	A	432	14.330	14.461	33.211	1.00	18.21
ATOM	2396	N	ASP	A	433	12.943	15.377	31.675	1.00	17.27
ATOM	2397	CA	ASP	A	433	12.202	16.253	32.589	1.00	16.24
ATOM	2398	CB	ASP	A	433	11.390	17.277	31.780	1.00	15.83
ATOM	2399	CG	ASP	A	433	10.417	18.084	32.631	1.00	15.05
ATOM	2400	OD1	ASP	A	433	10.656	18.266	33.846	1.00	16.45
ATOM	2401	OD2	ASP	A	433	9.382	18.592	32.154	1.00	13.26
ATOM	2402	C	ASP	A	433	11.304	15.488	33.569	1.00	15.99
ATOM	2403	O	ASP	A	433	10.463	14.668	33.167	1.00	15.55
ATOM	2404	N	THR	A	434	11.494	15.789	34.854	1.00	15.25
ATOM	2405	CA	THR	A	434	10.842	15.079	35.956	1.00	15.02
ATOM	2406	CB	THR	A	434	11.889	14.363	36.833	1.00	13.94
ATOM	2407	OG1	THR	A	434	13.013	15.232	37.035	1.00	13.12
ATOM	2408	CG2	THR	A	434	12.472	13.169	36.112	1.00	14.82
ATOM	2409	C	THR	A	434	10.095	16.058	36.836	1.00	13.54
ATOM	2410	O	THR	A	434	10.347	16.128	38.044	1.00	15.37
ATOM	2411	N	ARG	A	435	9.178	16.806	36.235	1.00	9.54
ATOM	2412	CA	ARG	A	435	8.452	17.836	36.953	1.00	7.55
ATOM	2413	CB	ARG	A	435	8.043	18.938	35.996	1.00	6.94
ATOM	2414	CG	ARG	A	435	6.838	18.596	35.163	1.00	8.64
ATOM	2415	CD	ARG	A	435	6.246	19.788	34.446	1.00	12.25
ATOM	2416	NE	ARG	A	435	7.084	20.172	33.320	1.00	11.98
ATOM	2417	CZ	ARG	A	435	7.706	21.325	33.213	1.00	10.79
ATOM	2418	NH1	ARG	A	435	7.581	22.243	34.160	1.00	10.79
ATOM	2419	NH2	ARG	A	435	8.453	21.559	32.146	1.00	12.40
ATOM	2420	C	ARG	A	435	7.232	17.285	37.669	1.00	11.60
ATOM	2421	O	ARG	A	435	6.531	18.030	38.352	1.00	14.72
ATOM	2422	N	TYR	A	436	6.980	15.984	37.505	1.00	14.41
ATOM	2423	CA	TYR	A	436	5.857	15.305	38.154	1.00	13.00
ATOM	2424	CB	TYR	A	436	4.899	14.750	37.101	1.00	12.31
ATOM	2425	CG	TYR	A	436	4.318	15.802	36.176	1.00	12.72
ATOM	2426	CD1	TYR	A	436	4.672	15.846	34.827	1.00	11.97
ATOM	2427	CE1	TYR	A	436	4.141	16.806	33.971	1.00	11.68
ATOM	2428	CZ	TYR	A	436	3.238	17.741	34.459	1.00	14.36
ATOM	2429	OH	TYR	A	436	2.695	18.702	33.613	1.00	14.60
ATOM	2430	CE2	TYR	A	436	2.871	17.717	35.802	1.00	15.32
ATOM	2431	CD2	TYR	A	436	3.414	16.750	36.648	1.00	13.69
ATOM	2432	C	TYR	A	436	6.332	14.204	39.114	1.00	15.33
ATOM	2433	O	TYR	A	436	5.645	13.192	39.338	1.00	17.52

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2434	N	PHE	A	437	7.516	14.411	39.688	1.00	14.74
ATOM	2435	CA	PHE	A	437	8.053	13.495	40.683	1.00	15.01
ATOM	2436	CB	PHE	A	437	9.177	12.652	40.088	1.00	9.23
ATOM	2437	CG	PHE	A	437	8.707	11.668	39.026	1.00	8.11
ATOM	2438	CD1	PHE	A	437	8.532	12.071	37.698	1.00	5.58
ATOM	2439	CE1	PHE	A	437	8.114	11.169	36.727	1.00	2.86
ATOM	2440	CZ	PHE	A	437	7.863	9.841	37.061	1.00	2.00
ATOM	2441	CE2	PHE	A	437	8.037	9.420	38.364	1.00	4.31
ATOM	2442	CD2	PHE	A	437	8.454	10.336	39.349	1.00	6.23
ATOM	2443	C	PHE	A	437	8.516	14.296	41.885	1.00	18.53
ATOM	2444	O	PHE	A	437	9.058	15.387	41.717	1.00	20.02
ATOM	2445	N	ASP	A	438	8.268	13.765	43.088	1.00	23.47
ATOM	2446	CA	ASP	A	438	8.584	14.449	44.352	1.00	26.09
ATOM	2447	CB	ASP	A	438	8.203	13.586	45.576	1.00	33.71
ATOM	2448	CG	ASP	A	438	6.727	13.763	46.016	1.00	42.00
ATOM	2449	OD1	ASP	A	438	5.954	12.763	45.994	1.00	46.17
ATOM	2450	OD2	ASP	A	438	6.249	14.853	46.417	1.00	43.62
ATOM	2451	C	ASP	A	438	10.065	14.819	44.403	1.00	23.94
ATOM	2452	O	ASP	A	438	10.940	13.982	44.155	1.00	21.39
ATOM	2453	N	GLU	A	439	10.334	16.083	44.705	1.00	22.31
ATOM	2454	CA	GLU	A	439	11.696	16.568	44.843	1.00	21.57
ATOM	2455	CB	GLU	A	439	11.698	18.076	45.063	1.00	25.90
ATOM	2456	CG	GLU	A	439	11.832	18.898	43.793	1.00	31.12
ATOM	2457	CD	GLU	A	439	11.707	20.389	44.062	1.00	35.66
ATOM	2458	OE1	GLU	A	439	10.769	20.784	44.793	1.00	37.72
ATOM	2459	OE2	GLU	A	439	12.543	21.172	43.551	1.00	38.40
ATOM	2460	C	GLU	A	439	12.448	15.858	45.977	1.00	19.40
ATOM	2461	O	GLU	A	439	13.677	15.817	45.979	1.00	18.71
ATOM	2462	N	GLU	A	440	11.717	15.300	46.938	1.00	17.67
ATOM	2463	CA	GLU	A	440	12.311	14.379	47.906	1.00	18.42
ATOM	2464	CB	GLU	A	440	11.219	13.697	48.746	1.00	23.20
ATOM	2465	CG	GLU	A	440	11.666	13.189	50.121	1.00	28.72
ATOM	2466	CD	GLU	A	440	11.089	11.819	50.505	1.00	31.66
ATOM	2467	OE1	GLU	A	440	9.896	11.554	50.212	1.00	32.34
ATOM	2468	OE2	GLU	A	440	11.828	11.002	51.120	1.00	32.38
ATOM	2469	C	GLU	A	440	13.180	13.324	47.196	1.00	17.00
ATOM	2470	O	GLU	A	440	14.143	12.818	47.765	1.00	15.43
ATOM	2471	N	PHE	A	441	12.849	13.010	45.946	1.00	18.63
ATOM	2472	CA	PHE	A	441	13.579	11.987	45.196	1.00	17.87
ATOM	2473	CB	PHE	A	441	12.622	10.924	44.659	1.00	15.69
ATOM	2474	CG	PHE	A	441	11.676	10.409	45.687	1.00	17.75
ATOM	2475	CD1	PHE	A	441	10.315	10.672	45.587	1.00	19.74
ATOM	2476	CE1	PHE	A	441	9.421	10.208	46.553	1.00	19.46
ATOM	2477	CZ	PHE	A	441	9.892	9.480	47.632	1.00	20.42
ATOM	2478	CE2	PHE	A	441	11.263	9.217	47.749	1.00	20.77
ATOM	2479	CD2	PHE	A	441	12.143	9.685	46.780	1.00	18.84
ATOM	2480	C	PHE	A	441	14.469	12.543	44.087	1.00	18.41
ATOM	2481	O	PHE	A	441	15.668	12.266	44.069	1.00	20.18
ATOM	2482	N	THR	A	442	13.894	13.324	43.175	1.00	16.17
ATOM	2483	CA	THR	A	442	14.655	13.854	42.044	1.00	14.82
ATOM	2484	CB	THR	A	442	13.771	14.728	41.153	1.00	15.66
ATOM	2485	OG1	THR	A	442	13.033	15.654	41.963	1.00	18.46

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2486	CG2	THR	A	442	12.697	13.874	40.496	1.00	15.68
ATOM	2487	C	THR	A	442	15.904	14.609	42.492	1.00	13.47
ATOM	2488	O	THR	A	442	17.020	14.289	42.063	1.00	11.96
ATOM	2489	N	ALA	A	443	15.696	15.581	43.380	1.00	12.58
ATOM	2490	CA	ALA	A	443	16.750	16.443	43.911	1.00	11.64
ATOM	2491	CB	ALA	A	443	16.172	17.421	44.922	1.00	11.16
ATOM	2492	C	ALA	A	443	17.925	15.684	44.519	1.00	11.90
ATOM	2493	O	ALA	A	443	19.050	16.139	44.409	1.00	11.09
ATOM	2494	N	GLN	A	444	17.656	14.535	45.144	1.00	15.91
ATOM	2495	CA	GLN	A	444	18.688	13.666	45.735	1.00	16.93
ATOM	2496	CB	GLN	A	444	18.089	12.333	46.216	1.00	17.44
ATOM	2497	CG	GLN	A	444	17.500	12.346	47.635	1.00	17.93
ATOM	2498	CD	GLN	A	444	17.325	10.948	48.230	1.00	17.80
ATOM	2499	OE1	GLN	A	444	16.255	10.610	48.747	1.00	16.82
ATOM	2500	NE2	GLN	A	444	18.379	10.140	48.168	1.00	18.55
ATOM	2501	C	GLN	A	444	19.785	13.371	44.733	1.00	17.83
ATOM	2502	O	GLN	A	444	19.510	13.175	43.552	1.00	17.46
ATOM	2503	N	SER	A	445	21.023	13.353	45.214	1.00	21.82
ATOM	2504	CA	SER	A	445	22.190	13.069	44.388	1.00	26.42
ATOM	2505	CB	SER	A	445	23.411	13.782	44.964	1.00	25.97
ATOM	2506	OG	SER	A	445	24.454	13.839	44.012	1.00	25.89
ATOM	2507	C	SER	A	445	22.419	11.562	44.360	1.00	30.03
ATOM	2508	O	SER	A	445	21.937	10.857	45.245	1.00	31.67
ATOM	2509	N	ILE	A	446	23.128	11.061	43.345	1.00	34.17
ATOM	2510	CA	ILE	A	446	23.424	9.617	43.253	1.00	37.93
ATOM	2511	CB	ILE	A	446	22.569	8.897	42.163	1.00	35.13
ATOM	2512	CG1	ILE	A	446	21.328	9.708	41.777	1.00	32.91
ATOM	2513	CD1	ILE	A	446	21.164	9.894	40.291	1.00	30.52
ATOM	2514	CG2	ILE	A	446	22.170	7.509	42.650	1.00	34.99
ATOM	2515	C	ILE	A	446	24.907	9.287	43.042	1.00	42.06
ATOM	2516	O	ILE	A	446	25.633	10.044	42.400	1.00	41.40
ATOM	2517	N	THR	A	447	25.337	8.143	43.581	1.00	48.62
ATOM	2518	CA	THR	A	447	26.705	7.641	43.393	1.00	54.23
ATOM	2519	CB	THR	A	447	27.181	6.806	44.630	1.00	54.12
ATOM	2520	OG1	THR	A	447	26.172	6.805	45.651	1.00	52.75
ATOM	2521	CG2	THR	A	447	28.386	7.470	45.306	1.00	52.75
ATOM	2522	C	THR	A	447	26.854	6.835	42.079	1.00	57.41
ATOM	2523	O	THR	A	447	26.590	5.620	42.044	1.00	57.99
ATOM	2524	N	ILE	A	448	27.271	7.530	41.011	1.00	58.95
ATOM	2525	CA	ILE	A	448	27.457	6.943	39.671	1.00	58.60
ATOM	2526	CB	ILE	A	448	27.233	8.021	38.532	1.00	59.46
ATOM	2527	CG1	ILE	A	448	26.874	7.352	37.188	1.00	58.50
ATOM	2528	CD1	ILE	A	448	26.212	8.285	36.155	1.00	55.93
ATOM	2529	CG2	ILE	A	448	28.448	8.978	38.402	1.00	59.54
ATOM	2530	C	ILE	A	448	28.822	6.264	39.533	1.00	56.94
ATOM	2531	O	ILE	A	448	29.744	6.536	40.303	1.00	54.73
TER	2531		ILE	A	448					
ATOM	2532	N	VAL	A	462	32.330	-14.621	42.822	1.00	29.03
ATOM	2533	CA	VAL	A	462	30.967	-14.453	42.328	1.00	31.88
ATOM	2534	CB	VAL	A	462	30.926	-14.299	40.778	1.00	32.80
ATOM	2535	CG1	VAL	A	462	29.568	-13.712	40.321	1.00	32.01
ATOM	2536	CG2	VAL	A	462	32.119	-13.448	40.260	1.00	32.03

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2537	C	VAL	A	462	30.056	-15.612	42.776	1.00	32.81
ATOM	2538	O	VAL	A	462	30.437	-16.786	42.649	1.00	35.61
ATOM	2539	N	ASP	A	463	28.866	-15.262	43.290	1.00	30.73
ATOM	2540	CA	ASP	A	463	27.848	-16.204	43.814	1.00	28.18
ATOM	2541	CB	ASP	A	463	27.822	-17.527	43.033	1.00	25.67
ATOM	2542	CG	ASP	A	463	27.038	-17.431	41.732	1.00	23.77
ATOM	2543	OD1	ASP	A	463	27.172	-16.426	40.995	1.00	23.24
ATOM	2544	OD2	ASP	A	463	26.261	-18.328	41.361	1.00	22.28
ATOM	2545	C	ASP	A	463	27.989	-16.446	45.327	1.00	28.40
ATOM	2546	O	ASP	A	463	28.787	-17.291	45.767	1.00	27.70
ATOM	2547	N	SER	A	464	27.171	-15.727	46.103	1.00	27.89
ATOM	2548	CA	SER	A	464	27.475	-15.425	47.510	1.00	26.48
ATOM	2549	CB	SER	A	464	27.780	-13.917	47.648	1.00	27.28
ATOM	2550	OG	SER	A	464	28.436	-13.593	48.867	1.00	27.64
ATOM	2551	C	SER	A	464	26.441	-15.853	48.563	1.00	23.91
ATOM	2552	O	SER	A	464	26.620	-15.558	49.747	1.00	24.37
ATOM	2553	N	GLU	A	465	25.381	-16.546	48.141	1.00	22.01
ATOM	2554	CA	GLU	A	465	24.335	-17.068	49.049	1.00	22.71
ATOM	2555	CB	GLU	A	465	24.930	-17.880	50.208	1.00	24.14
ATOM	2556	CG	GLU	A	465	23.903	-18.670	50.999	1.00	25.75
ATOM	2557	CD	GLU	A	465	23.477	-17.964	52.271	1.00	26.73
ATOM	2558	OE1	GLU	A	465	24.287	-17.933	53.226	1.00	26.40
ATOM	2559	OE2	GLU	A	465	22.334	-17.449	52.311	1.00	25.81
ATOM	2560	C	GLU	A	465	23.357	-16.007	49.570	1.00	22.06
ATOM	2561	O	GLU	A	465	22.144	-16.142	49.395	1.00	22.79
ATOM	2562	N	ARG	A	466	23.875	-14.968	50.225	1.00	21.00
ATOM	2563	CA	ARG	A	466	23.090	-13.744	50.429	1.00	19.59
ATOM	2564	CB	ARG	A	466	23.668	-12.844	51.540	1.00	20.63
ATOM	2565	CG	ARG	A	466	25.102	-12.317	51.322	1.00	20.37
ATOM	2566	CD	ARG	A	466	25.853	-11.926	52.610	1.00	18.99
ATOM	2567	NE	ARG	A	466	25.547	-12.813	53.736	1.00	18.72
ATOM	2568	CZ	ARG	A	466	25.981	-14.072	53.859	1.00	19.56
ATOM	2569	NH1	ARG	A	466	25.635	-14.786	54.922	1.00	18.24
ATOM	2570	NH2	ARG	A	466	26.759	-14.624	52.929	1.00	19.52
ATOM	2571	C	ARG	A	466	22.945	-12.988	49.100	1.00	16.56
ATOM	2572	O	ARG	A	466	21.963	-12.289	48.899	1.00	15.33
ATOM	2573	N	ARG	A	467	23.932	-13.153	48.211	1.00	14.83
ATOM	2574	CA	ARG	A	467	23.877	-12.704	46.815	1.00	11.72
ATOM	2575	CB	ARG	A	467	24.960	-11.654	46.510	1.00	14.84
ATOM	2576	CG	ARG	A	467	25.629	-10.995	47.694	1.00	20.60
ATOM	2577	CD	ARG	A	467	26.962	-10.343	47.339	1.00	27.04
ATOM	2578	NE	ARG	A	467	27.371	-9.341	48.325	1.00	32.91
ATOM	2579	CZ	ARG	A	467	27.067	-8.042	48.266	1.00	35.36
ATOM	2580	NH1	ARG	A	467	26.344	-7.558	47.265	1.00	36.83
ATOM	2581	NH2	ARG	A	467	27.490	-7.218	49.217	1.00	36.43
ATOM	2582	C	ARG	A	467	24.014	-13.866	45.804	1.00	8.55
ATOM	2583	O	ARG	A	467	25.040	-13.979	45.117	1.00	7.15
ATOM	2584	N	PRO	A	468	22.979	-14.698	45.675	1.00	5.25
ATOM	2585	CA	PRO	A	468	23.043	-15.872	44.798	1.00	4.79
ATOM	2586	CB	PRO	A	468	21.948	-16.772	45.365	1.00	4.41
ATOM	2587	CG	PRO	A	468	20.929	-15.815	45.880	1.00	4.60
ATOM	2588	CD	PRO	A	468	21.657	-14.571	46.313	1.00	3.51

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2589	C	PRO	A	468	22.726	-15.516	43.344	1.00	4.93
ATOM	2590	O	PRO	A	468	22.462	-14.355	43.036	1.00	7.95
ATOM	2591	N	HIS	A	469	22.765	-16.507	42.460	1.00	2.40
ATOM	2592	CA	HIS	A	469	22.336	-16.327	41.082	1.00	2.00
ATOM	2593	CB	HIS	A	469	22.892	-17.446	40.223	1.00	2.00
ATOM	2594	CG	HIS	A	469	22.596	-17.304	38.766	1.00	2.00
ATOM	2595	ND1	HIS	A	469	22.981	-16.204	38.031	1.00	2.00
ATOM	2596	CE1	HIS	A	469	22.605	-16.365	36.775	1.00	2.27
ATOM	2597	NE2	HIS	A	469	21.994	-17.531	36.669	1.00	2.42
ATOM	2598	CD2	HIS	A	469	21.981	-18.141	37.898	1.00	2.00
ATOM	2599	C	HIS	A	469	20.848	-16.454	41.088	1.00	3.01
ATOM	2600	O	HIS	A	469	20.291	-17.126	41.952	1.00	8.45
ATOM	2601	N	PHE	A	470	20.189	-15.799	40.143	1.00	3.70
ATOM	2602	CA	PHE	A	470	18.764	-16.017	39.940	1.00	2.31
ATOM	2603	CB	PHE	A	470	18.002	-14.697	39.995	1.00	2.00
ATOM	2604	CG	PHE	A	470	17.943	-14.083	41.373	1.00	2.00
ATOM	2605	CD1	PHE	A	470	16.731	-13.955	42.040	1.00	2.82
ATOM	2606	CE1	PHE	A	470	16.659	-13.393	43.293	1.00	2.00
ATOM	2607	CZ	PHE	A	470	17.796	-12.954	43.907	1.00	2.00
ATOM	2608	CE2	PHE	A	470	19.013	-13.071	43.267	1.00	2.75
ATOM	2609	CD2	PHE	A	470	19.085	-13.625	42.000	1.00	2.00
ATOM	2610	C	PHE	A	470	18.637	-16.696	38.587	1.00	3.26
ATOM	2611	O	PHE	A	470	18.889	-16.079	37.561	1.00	7.10
ATOM	2612	N	PRO	A	471	18.346	-17.991	38.583	1.00	2.89
ATOM	2613	CA	PRO	A	471	18.218	-18.740	37.333	1.00	3.97
ATOM	2614	CB	PRO	A	471	17.851	-20.153	37.812	1.00	6.10
ATOM	2615	CG	PRO	A	471	18.398	-20.231	39.201	1.00	4.25
ATOM	2616	CD	PRO	A	471	18.171	-18.856	39.763	1.00	4.21
ATOM	2617	C	PRO	A	471	17.121	-18.182	36.437	1.00	4.41
ATOM	2618	O	PRO	A	471	16.034	-17.864	36.935	1.00	2.00
ATOM	2619	N	GLN	A	472	17.428	-18.056	35.142	1.00	6.75
ATOM	2620	CA	GLN	A	472	16.458	-17.674	34.109	1.00	10.11
ATOM	2621	CB	GLN	A	472	15.492	-18.834	33.778	1.00	14.63
ATOM	2622	CG	GLN	A	472	16.071	-20.254	33.857	1.00	18.29
ATOM	2623	CD	GLN	A	472	16.974	-20.597	32.678	1.00	20.73
ATOM	2624	OE1	GLN	A	472	18.198	-20.435	32.753	1.00	22.50
ATOM	2625	NE2	GLN	A	472	16.376	-21.077	31.592	1.00	21.17
ATOM	2626	C	GLN	A	472	15.670	-16.426	34.512	1.00	10.43
ATOM	2627	O	GLN	A	472	14.431	-16.428	34.542	1.00	11.93
ATOM	2628	N	PHE	A	473	16.403	-15.363	34.823	1.00	8.38
ATOM	2629	CA	PHE	A	473	15.822	-14.135	35.341	1.00	6.25
ATOM	2630	CB	PHE	A	473	16.553	-13.749	36.626	1.00	4.31
ATOM	2631	CG	PHE	A	473	16.182	-12.414	37.189	1.00	5.05
ATOM	2632	CD1	PHE	A	473	15.150	-12.300	38.110	1.00	6.22
ATOM	2633	CE1	PHE	A	473	14.822	-11.059	38.665	1.00	6.94
ATOM	2634	CZ	PHE	A	473	15.538	-9.922	38.303	1.00	6.54
ATOM	2635	CE2	PHE	A	473	16.588	-10.023	37.386	1.00	5.98
ATOM	2636	CD2	PHE	A	473	16.910	-11.268	36.847	1.00	6.62
ATOM	2637	C	PHE	A	473	15.943	-13.073	34.259	1.00	8.33
ATOM	2638	O	PHE	A	473	14.999	-12.330	34.002	1.00	8.66
ATOM	2639	N	ASP	A	474	17.093	-13.038	33.596	1.00	10.32
ATOM	2640	CA	ASP	A	474	17.351	-12.049	32.556	1.00	13.73

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2641	CB	ASP	A	474	18.824	-12.079	32.147	1.00	19.99
ATOM	2642	CG	ASP	A	474	19.756	-11.804	33.322	1.00	25.09
ATOM	2643	OD1	ASP	A	474	19.758	-12.626	34.267	1.00	27.20
ATOM	2644	OD2	ASP	A	474	20.508	-10.800	33.400	1.00	26.77
ATOM	2645	C	ASP	A	474	16.434	-12.183	31.342	1.00	11.65
ATOM	2646	O	ASP	A	474	16.105	-13.282	30.921	1.00	12.33
ATOM	2647	N	TYR	A	475	16.027	-11.043	30.797	1.00	10.82
ATOM	2648	CA	TYR	A	475	15.051	-10.982	29.724	1.00	10.43
ATOM	2649	CB	TYR	A	475	13.643	-11.008	30.316	1.00	9.78
ATOM	2650	CG	TYR	A	475	12.552	-10.481	29.404	1.00	8.52
ATOM	2651	CD1	TYR	A	475	11.808	-11.347	28.607	1.00	8.82
ATOM	2652	CE1	TYR	A	475	10.810	-10.878	27.772	1.00	9.06
ATOM	2653	CZ	TYR	A	475	10.539	-9.525	27.730	1.00	9.88
ATOM	2654	OH	TYR	A	475	9.536	-9.060	26.906	1.00	12.39
ATOM	2655	CE2	TYR	A	475	11.257	-8.642	28.517	1.00	9.17
ATOM	2656	CD2	TYR	A	475	12.255	-9.123	29.349	1.00	8.01
ATOM	2657	C	TYR	A	475	15.221	-9.708	28.910	1.00	14.83
ATOM	2658	O	TYR	A	475	15.369	-8.619	29.473	1.00	15.48
ATOM	2659	N	SER	A	476	15.177	-9.854	27.586	1.00	19.52
ATOM	2660	CA	SER	A	476	15.089	-8.715	26.668	1.00	22.51
ATOM	2661	CB	SER	A	476	16.444	-8.450	26.012	1.00	23.32
ATOM	2662	OG	SER	A	476	17.410	-8.139	27.001	1.00	24.41
ATOM	2663	C	SER	A	476	13.977	-8.894	25.617	1.00	23.84
ATOM	2664	O	SER	A	476	13.631	-10.021	25.249	1.00	23.58
ATOM	2665	N	ALA	A	477	13.419	-7.778	25.151	1.00	25.99
ATOM	2666	CA	ALA	A	477	12.286	-7.797	24.228	1.00	29.87
ATOM	2667	CB	ALA	A	477	11.243	-6.792	24.669	1.00	31.38
ATOM	2668	C	ALA	A	477	12.698	-7.538	22.783	1.00	32.99
ATOM	2669	O	ALA	A	477	13.846	-7.193	22.512	1.00	31.52
ATOM	2670	N	SER	A	478	11.742	-7.678	21.867	1.00	39.23
ATOM	2671	CA	SER	A	478	12.006	-7.640	20.422	1.00	46.05
ATOM	2672	CB	SER	A	478	10.852	-8.300	19.651	1.00	45.56
ATOM	2673	OG	SER	A	478	10.801	-9.695	19.899	1.00	44.26
ATOM	2674	C	SER	A	478	12.338	-6.259	19.815	1.00	51.01
ATOM	2675	O	SER	A	478	12.290	-6.100	18.587	1.00	50.93
ATOM	2676	N	SER	A	479	12.660	-5.281	20.674	1.00	56.07
ATOM	2677	CA	SER	A	479	13.231	-3.970	20.285	1.00	60.50
ATOM	2678	CB	SER	A	479	13.264	-3.758	18.760	1.00	59.31
ATOM	2679	OG	SER	A	479	14.507	-4.167	18.209	1.00	57.46
ATOM	2680	C	SER	A	479	12.581	-2.758	20.966	1.00	64.42
ATOM	2681	O	SER	A	479	13.285	-1.844	21.415	1.00	66.04
ATOM	2682	N	THR	A	480	11.249	-2.744	21.029	1.00	68.01
ATOM	2683	CA	THR	A	480	10.518	-1.591	21.569	1.00	70.48
ATOM	2684	CB	THR	A	480	9.611	-0.907	20.477	1.00	71.90
ATOM	2685	OG1	THR	A	480	8.389	-1.644	20.317	1.00	73.01
ATOM	2686	CG2	THR	A	480	10.254	-0.962	19.073	1.00	71.50
ATOM	2687	C	THR	A	480	9.702	-1.954	22.814	1.00	70.06
ATOM	2688	O	THR	A	480	8.828	-2.825	22.766	1.00	70.83
ATOM	2689	N	ALA	A	481	10.012	-1.293	23.927	1.00	68.83
ATOM	2690	CA	ALA	A	481	9.262	-1.452	25.171	1.00	67.76
ATOM	2691	CB	ALA	A	481	9.639	-2.741	25.876	1.00	65.66
ATOM	2692	C	ALA	A	481	9.496	-0.254	26.081	1.00	69.28

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2693	O	ALA	A	481	9.867	0.826	25.618	1.00	71.43
TER PEPTIDE A										
ATOM	2694	N	GLY	A	3	-2.454	15.839	53.220	1.00	59.77
ATOM	2695	CA	GLY	A	3	-3.404	14.806	52.720	1.00	63.34
ATOM	2696	C	GLY	A	3	-2.775	13.431	52.602	1.00	65.23
ATOM	2697	O	GLY	A	3	-2.205	13.082	51.558	1.00	68.14
ATOM	2698	N	ARG	A	4	-2.905	12.652	53.676	1.00	64.00
ATOM	2699	CA	ARG	A	4	-2.278	11.329	53.831	1.00	61.26
ATOM	2700	CB	ARG	A	4	-3.188	10.206	53.324	1.00	57.91
ATOM	2701	CG	ARG	A	4	-3.107	9.935	51.850	1.00	56.34
ATOM	2702	CD	ARG	A	4	-3.517	8.535	51.482	1.00	53.99
ATOM	2703	NE	ARG	A	4	-2.387	7.755	51.012	1.00	51.59
ATOM	2704	CZ	ARG	A	4	-2.022	7.650	49.746	1.00	51.26
ATOM	2705	NH1	ARG	A	4	-2.695	8.269	48.792	1.00	51.55
ATOM	2706	NH2	ARG	A	4	-0.974	6.919	49.429	1.00	53.20
ATOM	2707	C	ARG	A	4	-0.825	11.159	53.329	1.00	60.21
ATOM	2708	O	ARG	A	4	-0.520	11.333	52.133	1.00	59.47
ATOM	2709	N	PRO	A	5	0.055	10.809	54.268	1.00	56.58
ATOM	2710	CA	PRO	A	5	1.437	10.453	53.966	1.00	53.20
ATOM	2711	CB	PRO	A	5	1.967	10.013	55.330	1.00	55.07
ATOM	2712	CG	PRO	A	5	0.736	9.598	56.070	1.00	56.56
ATOM	2713	CD	PRO	A	5	-0.212	10.707	55.712	1.00	56.60
ATOM	2714	C	PRO	A	5	1.517	9.272	53.014	1.00	51.17
ATOM	2715	O	PRO	A	5	0.730	8.327	53.097	1.00	52.66
ATOM	2716	N	ARG	A	6	2.480	9.351	52.113	1.00	49.43
ATOM	2717	CA	ARG	A	6	2.923	8.231	51.305	1.00	49.47
ATOM	2718	CB	ARG	A	6	4.294	8.566	50.762	1.00	45.72
ATOM	2719	CG	ARG	A	6	4.819	7.592	49.784	1.00	49.30
ATOM	2720	CD	ARG	A	6	5.554	8.271	48.692	1.00	52.59
ATOM	2721	NE	ARG	A	6	5.891	7.368	47.610	1.00	54.37
ATOM	2722	CZ	ARG	A	6	6.057	7.781	46.376	1.00	57.39
ATOM	2723	NH1	ARG	A	6	5.899	9.077	46.104	1.00	58.86
ATOM	2724	NH2	ARG	A	6	6.375	6.915	45.420	1.00	58.53
ATOM	2725	C	ARG	A	6	3.004	6.909	52.084	1.00	53.73
ATOM	2726	O	ARG	A	6	3.533	6.858	53.202	1.00	56.89
ATOM	2727	N	THR	A	7	2.487	5.846	51.469	1.00	54.48
ATOM	2728	CA	THR	A	7	2.452	4.511	52.059	1.00	53.43
ATOM	2729	CB	THR	A	7	1.040	3.922	51.913	1.00	54.97
ATOM	2730	OG1	THR	A	7	0.805	3.582	50.538	1.00	55.62
ATOM	2731	CG2	THR	A	7	-0.017	4.977	52.190	1.00	54.48
ATOM	2732	C	THR	A	7	3.437	3.602	51.343	1.00	52.28
ATOM	2733	O	THR	A	7	3.782	3.861	50.185	1.00	54.07
ATOM	2734	N	THR	A	8	3.893	2.549	52.025	1.00	49.53
ATOM	2735	CA	THR	A	8	4.673	1.494	51.366	1.00	51.75
ATOM	2736	CB	THR	A	8	6.169	1.497	51.773	1.00	55.90
ATOM	2737	OG1	THR	A	8	6.272	1.356	53.195	1.00	59.32
ATOM	2738	CG2	THR	A	8	6.879	2.860	51.437	1.00	57.69
ATOM	2739	C	THR	A	8	4.060	0.150	51.685	1.00	48.28
ATOM	2740	O	THR	A	8	3.385	0.014	52.698	1.00	53.43
ATOM	2741	N	SER	A	9	4.312	-0.837	50.828	1.00	42.88
ATOM	2742	CA	SER	A	9	3.671	-2.141	50.918	1.00	37.85
ATOM	2743	CB	SER	A	9	3.649	-2.790	49.541	1.00	39.65

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2744	OG	SER	A	9	4.938	-3.228	49.167	1.00	41.04
ATOM	2745	C	SER	A	9	4.350	-3.069	51.920	1.00	36.94
ATOM	2746	O	SER	A	9	5.337	-2.705	52.543	1.00	35.22
ATOM	2747	N	PHE	A	10	3.823	-4.277	52.070	1.00	37.43
ATOM	2748	CA	PHE	A	10	4.352	-5.198	53.054	1.00	41.36
ATOM	2749	CB	PHE	A	10	3.849	-4.798	54.449	1.00	43.51
ATOM	2750	CG	PHE	A	10	2.418	-5.165	54.699	1.00	47.05
ATOM	2751	CD1	PHE	A	10	2.088	-6.411	55.240	1.00	49.04
ATOM	2752	CE1	PHE	A	10	0.756	-6.773	55.446	1.00	50.01
ATOM	2753	CZ	PHE	A	10	-0.263	-5.882	55.116	1.00	49.88
ATOM	2754	CE2	PHE	A	10	0.054	-4.633	54.577	1.00	48.79
ATOM	2755	CD2	PHE	A	10	1.392	-4.284	54.372	1.00	48.20
ATOM	2756	C	PHE	A	10	3.929	-6.625	52.720	1.00	46.07
ATOM	2757	O	PHE	A	10	2.993	-6.808	51.924	1.00	41.79
ATOM	2758	N	ALA	A	11	4.615	-7.609	53.337	1.00	52.65
ATOM	2759	CA	ALA	A	11	4.234	-9.042	53.308	1.00	57.70
ATOM	2760	CB	ALA	A	11	4.770	-9.730	52.049	1.00	55.58
ATOM	2761	C	ALA	A	11	4.631	-9.858	54.562	1.00	62.68
ATOM	2762	O	ALA	A	11	5.822	-10.062	54.839	1.00	63.97
ATOM	2763	N	GLU	A	12	3.620	-10.333	55.297	1.00	67.34
ATOM	2764	CA	GLU	A	12	3.793	-11.258	56.425	1.00	68.21
ATOM	2765	CB	GLU	A	12	2.461	-11.451	57.184	1.00	72.49
ATOM	2766	CG	GLU	A	12	2.570	-11.968	58.629	1.00	79.61
ATOM	2767	CD	GLU	A	12	1.320	-12.729	59.136	1.00	84.11
ATOM	2768	OE1	GLU	A	12	0.656	-12.247	60.096	1.00	83.62
ATOM	2769	OE2	GLU	A	12	1.000	-13.827	58.599	1.00	86.05
ATOM	2770	C	GLU	A	12	4.277	-12.593	55.874	1.00	67.02
ATOM	2771	O	GLU	A	12	3.586	-13.230	55.074	1.00	65.82
TER Nucleotide A										
ATOM	2772	O1A	ANP	A	490	7.746	-0.022	41.698	1.00	35.93
ATOM	2773	PA	ANP	A	490	7.806	0.868	43.030	1.00	35.16
ATOM	2774	O2A	ANP	A	490	6.367	1.219	43.604	1.00	35.78
ATOM	2775	O3A	ANP	A	490	8.781	0.266	44.165	1.00	38.17
ATOM	2776	PB	ANP	A	490	8.219	-0.290	45.557	1.00	39.61
ATOM	2777	O1B	ANP	A	490	9.354	-0.331	46.671	1.00	40.09
ATOM	2778	O2B	ANP	A	490	7.590	-1.715	45.264	1.00	36.29
ATOM	2779	N3B	ANP	A	490	6.945	0.666	46.231	1.00	40.41
ATOM	2780	PG	ANP	A	490	5.885	-0.321	47.201	1.00	38.25
ATOM	2781	O3G	ANP	A	490	6.411	-0.345	48.702	1.00	40.92
ATOM	2782	O2G	ANP	A	490	4.430	0.307	47.167	1.00	41.75
ATOM	2783	O1G	ANP	A	490	5.861	-1.782	46.588	1.00	36.72
ATOM	2784	O5*	ANP	A	490	8.626	2.195	42.741	1.00	31.73
ATOM	2785	C5*	ANP	A	490	8.678	3.206	43.722	1.00	31.76
ATOM	2786	C4*	ANP	A	490	8.277	4.427	42.929	1.00	34.78
ATOM	2787	O4*	ANP	A	490	9.086	4.561	41.750	1.00	32.89
ATOM	2788	C1*	ANP	A	490	8.359	5.295	40.754	1.00	33.06
ATOM	2789	C2*	ANP	A	490	6.957	5.486	41.331	1.00	34.08
ATOM	2790	O2*	ANP	A	490	6.908	6.784	41.926	1.00	33.18
ATOM	2791	C3*	ANP	A	490	6.856	4.368	42.365	1.00	34.86
ATOM	2792	O3*	ANP	A	490	5.811	4.487	43.339	1.00	34.01
ATOM	2793	N9	ANP	A	490	8.269	4.512	39.496	1.00	29.79
ATOM	2794	C8	ANP	A	490	8.077	3.187	39.400	1.00	30.79

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2795	N7	ANP	A	490	8.014	2.738	38.116	1.00	30.51
ATOM	2796	C5	ANP	A	490	8.175	3.806	37.348	1.00	31.16
ATOM	2797	C6	ANP	A	490	8.219	4.114	35.903	1.00	35.88
ATOM	2798	N6	ANP	A	490	8.072	3.103	35.010	1.00	40.38
ATOM	2799	C4	ANP	A	490	8.330	4.917	38.249	1.00	28.69
ATOM	2800	N3	ANP	A	490	8.504	6.239	37.747	1.00	30.51
ATOM	2801	C2	ANP	A	490	8.528	6.395	36.411	1.00	35.81
ATOM	2802	N1	ANP	A	490	8.399	5.394	35.509	1.00	34.95
ATOM	2803	MN	MN	A	491	4.819	1.152	44.653	1.00	35.84
ATOM	2804	MN	MN	A	492	5.692	-2.995	45.330	1.00	52.47
TER										
ATOM	2805	O	HOH	A	500	4.426	12.104	51.909	1.00	42.36
ATOM	2806	O	HOH	A	501	5.627	-13.477	51.544	1.00	35.43
ATOM	2807	O	HOH	A	502	11.354	-15.784	49.503	1.00	38.30
ATOM	2808	O	HOH	A	503	-2.804	12.308	48.376	1.00	27.45
ATOM	2809	O	HOH	A	504	0.959	1.839	63.849	1.00	31.25
ATOM	2810	O	HOH	A	505	-16.543	-0.308	53.597	1.00	29.80
ATOM	2811	O	HOH	A	506	2.705	-16.629	29.426	1.00	65.56
ATOM	2812	O	HOH	A	507	-5.035	12.206	32.492	1.00	37.82
ATOM	2813	O	HOH	A	508	20.328	-18.653	33.701	1.00	31.39
ATOM	2814	O	HOH	A	509	7.557	-11.808	52.321	1.00	49.98
ATOM	2815	O	HOH	A	510	6.457	-5.738	48.691	1.00	32.48
ATOM	2816	O	HOH	A	511	2.515	-14.181	34.209	1.00	52.27
ATOM	2817	O	HOH	A	512	0.867	3.100	56.892	1.00	51.11
ATOM	2818	O	HOH	A	513	7.998	10.436	43.186	1.00	51.40
ATOM	2819	O	HOH	A	514	-6.287	-4.147	48.669	1.00	42.79
ATOM	2820	O	HOH	A	515	-7.047	10.124	53.539	1.00	16.21
ATOM	2821	O	HOH	A	516	-14.864	14.377	52.119	1.00	27.95
ATOM	2822	O	HOH	A	517	-20.995	-0.876	51.272	1.00	41.50
ATOM	2823	O	HOH	A	518	7.067	-2.676	38.556	1.00	52.19

FIGURE 3 (Cont.)

Molecule B

	A	B	C	D	E	F	G	H	I	J
ATOM	2824	N	PRO	B	141	55.967	72.234	-24.377	1.00	25.65
ATOM	2825	CA	PRO	B	141	55.049	72.260	-23.201	1.00	26.88
ATOM	2826	CB	PRO	B	141	55.076	73.733	-22.789	1.00	25.75
ATOM	2827	CG	PRO	B	141	56.468	74.185	-23.160	1.00	25.49
ATOM	2828	CD	PRO	B	141	56.930	73.348	-24.341	1.00	25.20
ATOM	2829	C	PRO	B	141	53.621	71.815	-23.540	1.00	28.46
ATOM	2830	O	PRO	B	141	53.285	71.695	-24.722	1.00	27.28
ATOM	2831	N	LYS	B	142	52.822	71.561	-22.497	1.00	30.99
ATOM	2832	CA	LYS	B	142	51.411	71.127	-22.581	1.00	33.92
ATOM	2833	CB	LYS	B	142	50.752	71.575	-23.898	1.00	34.19
ATOM	2834	CG	LYS	B	142	49.419	72.286	-23.721	1.00	34.83
ATOM	2835	CD	LYS	B	142	48.260	71.431	-24.227	1.00	35.69
ATOM	2836	CE	LYS	B	142	47.565	70.663	-23.100	1.00	36.71
ATOM	2837	NZ	LYS	B	142	47.239	69.250	-23.472	1.00	36.54

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2838	C	LYS	B	142	51.214	69.613	-22.350	1.00	35.24
ATOM	2839	O	LYS	B	142	51.927	68.800	-22.945	1.00	34.48
ATOM	2840	N	HIS	B	143	50.253	69.245	-21.490	1.00	37.31
ATOM	2841	CA	HIS	B	143	49.964	67.826	-21.194	1.00	39.24
ATOM	2842	CB	HIS	B	143	50.710	67.363	-19.932	1.00	41.24
ATOM	2843	CG	HIS	B	143	51.251	65.965	-20.025	1.00	44.44
ATOM	2844	ND1	HIS	B	143	51.391	65.144	-18.924	1.00	46.18
ATOM	2845	CE1	HIS	B	143	51.892	63.981	-19.302	1.00	46.30
ATOM	2846	NE2	HIS	B	143	52.082	64.015	-20.610	1.00	45.69
ATOM	2847	CD2	HIS	B	143	51.690	65.243	-21.086	1.00	44.97
ATOM	2848	C	HIS	B	143	48.476	67.433	-21.098	1.00	38.35
ATOM	2849	O	HIS	B	143	47.621	68.271	-20.809	1.00	38.18
ATOM	2850	N	ARG	B	144	48.200	66.147	-21.346	1.00	37.37
ATOM	2851	CA	ARG	B	144	46.856	65.548	-21.278	1.00	36.93
ATOM	2852	CB	ARG	B	144	46.766	64.340	-22.219	1.00	36.20
ATOM	2853	CG	ARG	B	144	47.820	63.253	-21.961	1.00	35.57
ATOM	2854	CD	ARG	B	144	47.789	62.084	-22.941	1.00	35.98
ATOM	2855	NE	ARG	B	144	48.217	62.478	-24.286	1.00	37.34
ATOM	2856	CZ	ARG	B	144	48.164	61.698	-25.366	1.00	36.61
ATOM	2857	NH1	ARG	B	144	47.699	60.456	-25.285	1.00	36.43
ATOM	2858	NH2	ARG	B	144	48.581	62.163	-26.537	1.00	35.98
ATOM	2859	C	ARG	B	144	46.519	65.118	-19.848	1.00	38.00
ATOM	2860	O	ARG	B	144	47.303	65.382	-18.933	1.00	38.83
ATOM	2861	N	VAL	B	145	45.375	64.448	-19.650	1.00	37.99
ATOM	2862	CA	VAL	B	145	44.955	64.046	-18.293	1.00	37.66
ATOM	2863	CB	VAL	B	145	44.719	65.320	-17.391	1.00	37.43
ATOM	2864	CG1	VAL	B	145	43.250	65.763	-17.377	1.00	36.42
ATOM	2865	CG2	VAL	B	145	45.284	65.120	-15.979	1.00	37.58
ATOM	2866	C	VAL	B	145	43.778	63.042	-18.151	1.00	37.36
ATOM	2867	O	VAL	B	145	43.537	62.531	-17.056	1.00	36.86
ATOM	2868	N	THR	B	146	43.078	62.732	-19.242	1.00	38.07
ATOM	2869	CA	THR	B	146	41.789	62.018	-19.153	1.00	38.65
ATOM	2870	CB	THR	B	146	40.933	62.183	-20.456	1.00	41.17
ATOM	2871	OG1	THR	B	146	41.544	63.128	-21.350	1.00	42.20
ATOM	2872	CG2	THR	B	146	39.577	62.826	-20.128	1.00	41.16
ATOM	2873	C	THR	B	146	41.845	60.545	-18.702	1.00	37.11
ATOM	2874	O	THR	B	146	42.919	59.946	-18.627	1.00	34.40
ATOM	2875	N	MET	B	147	40.656	59.984	-18.460	1.00	38.23
ATOM	2876	CA	MET	B	147	40.422	58.784	-17.632	1.00	39.19
ATOM	2877	CB	MET	B	147	38.932	58.715	-17.230	1.00	41.33
ATOM	2878	CG	MET	B	147	38.504	57.476	-16.419	1.00	43.05
ATOM	2879	SD	MET	B	147	38.486	57.722	-14.614	1.00	45.63
ATOM	2880	CE	MET	B	147	36.884	57.098	-14.165	1.00	44.48
ATOM	2881	C	MET	B	147	40.892	57.404	-18.125	1.00	37.93
ATOM	2882	O	MET	B	147	41.692	56.757	-17.446	1.00	38.55
ATOM	2883	N	ASN	B	148	40.377	56.934	-19.262	1.00	35.19
ATOM	2884	CA	ASN	B	148	40.535	55.519	-19.627	1.00	32.46
ATOM	2885	CB	ASN	B	148	39.451	55.070	-20.624	1.00	31.08
ATOM	2886	CG	ASN	B	148	39.757	55.477	-22.053	1.00	30.50
ATOM	2887	OD1	ASN	B	148	40.143	54.647	-22.877	1.00	28.96
ATOM	2888	ND2	ASN	B	148	39.579	56.756	-22.356	1.00	30.60
ATOM	2889	C	ASN	B	148	41.947	55.081	-20.053	1.00	31.76

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2890	O	ASN	B	148	42.118	54.069	-20.737	1.00	31.62
ATOM	2891	N	GLU	B	149	42.952	55.840	-19.620	1.00	31.55
ATOM	2892	CA	GLU	B	149	44.352	55.446	-19.761	1.00	32.79
ATOM	2893	CB	GLU	B	149	45.245	56.683	-19.860	1.00	34.53
ATOM	2894	CG	GLU	B	149	46.360	56.547	-20.886	1.00	38.42
ATOM	2895	CD	GLU	B	149	46.896	57.887	-21.354	1.00	40.44
ATOM	2896	OE1	GLU	B	149	47.234	58.008	-22.560	1.00	39.02
ATOM	2897	OE2	GLU	B	149	46.979	58.816	-20.512	1.00	41.25
ATOM	2898	C	GLU	B	149	44.795	54.547	-18.596	1.00	32.34
ATOM	2899	O	GLU	B	149	45.989	54.428	-18.296	1.00	32.04
ATOM	2900	N	PHE	B	150	43.815	53.920	-17.946	1.00	31.13
ATOM	2901	CA	PHE	B	150	44.045	53.030	-16.816	1.00	29.14
ATOM	2902	CB	PHE	B	150	43.658	53.726	-15.513	1.00	26.42
ATOM	2903	CG	PHE	B	150	44.526	54.897	-15.165	1.00	24.27
ATOM	2904	CD1	PHE	B	150	45.637	54.732	-14.342	1.00	24.17
ATOM	2905	CE1	PHE	B	150	46.443	55.818	-14.009	1.00	23.48
ATOM	2906	CZ	PHE	B	150	46.135	57.086	-14.502	1.00	22.82
ATOM	2907	CE2	PHE	B	150	45.022	57.260	-15.318	1.00	21.75
ATOM	2908	CD2	PHE	B	150	44.224	56.169	-15.640	1.00	22.24
ATOM	2909	C	PHE	B	150	43.204	51.770	-16.966	1.00	30.40
ATOM	2910	O	PHE	B	150	42.017	51.850	-17.292	1.00	30.97
ATOM	2911	N	GLU	B	151	43.820	50.612	-16.738	1.00	32.16
ATOM	2912	CA	GLU	B	151	43.083	49.346	-16.645	1.00	33.17
ATOM	2913	CB	GLU	B	151	43.803	48.197	-17.380	1.00	33.04
ATOM	2914	CG	GLU	B	151	45.164	47.805	-16.816	1.00	32.26
ATOM	2915	CD	GLU	B	151	45.949	46.896	-17.739	1.00	31.33
ATOM	2916	OE1	GLU	B	151	46.934	47.366	-18.347	1.00	30.58
ATOM	2917	OE2	GLU	B	151	45.581	45.708	-17.852	1.00	31.56
ATOM	2918	C	GLU	B	151	42.789	48.999	-15.175	1.00	32.79
ATOM	2919	O	GLU	B	151	43.661	49.116	-14.304	1.00	31.86
ATOM	2920	N	TYR	B	152	41.546	48.599	-14.912	1.00	31.61
ATOM	2921	CA	TYR	B	152	41.065	48.387	-13.549	1.00	29.61
ATOM	2922	CB	TYR	B	152	39.673	49.013	-13.354	1.00	27.68
ATOM	2923	CG	TYR	B	152	39.522	50.419	-13.917	1.00	25.99
ATOM	2924	CD1	TYR	B	152	40.629	51.256	-14.072	1.00	26.09
ATOM	2925	CE1	TYR	B	152	40.507	52.533	-14.590	1.00	25.95
ATOM	2926	CZ	TYR	B	152	39.265	53.006	-14.953	1.00	26.19
ATOM	2927	OH	TYR	B	152	39.171	54.281	-15.462	1.00	26.39
ATOM	2928	CE2	TYR	B	152	38.136	52.205	-14.806	1.00	25.84
ATOM	2929	CD2	TYR	B	152	38.272	50.914	-14.290	1.00	25.38
ATOM	2930	C	TYR	B	152	41.059	46.897	-13.230	1.00	29.35
ATOM	2931	O	TYR	B	152	40.402	46.105	-13.913	1.00	30.27
ATOM	2932	N	LEU	B	153	41.802	46.528	-12.190	1.00	27.64
ATOM	2933	CA	LEU	B	153	42.066	45.129	-11.874	1.00	25.68
ATOM	2934	CB	LEU	B	153	43.546	44.947	-11.524	1.00	25.67
ATOM	2935	CG	LEU	B	153	44.573	44.871	-12.656	1.00	24.65
ATOM	2936	CD1	LEU	B	153	44.915	46.246	-13.211	1.00	23.31
ATOM	2937	CD2	LEU	B	153	45.830	44.181	-12.146	1.00	26.63
ATOM	2938	C	LEU	B	153	41.190	44.609	-10.734	1.00	24.16
ATOM	2939	O	LEU	B	153	40.482	43.608	-10.887	1.00	23.10
ATOM	2940	N	LYS	B	154	41.250	45.293	-9.592	1.00	21.85
ATOM	2941	CA	LYS	B	154	40.504	44.889	-8.404	1.00	18.64

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2942	CB	LYS	B	154	41.378	44.013	-7.495	1.00	18.98
ATOM	2943	CG	LYS	B	154	41.555	42.579	-7.970	1.00	18.54
ATOM	2944	CD	LYS	B	154	42.147	41.711	-6.880	1.00	18.55
ATOM	2945	CE	LYS	B	154	43.487	41.140	-7.301	1.00	19.63
ATOM	2946	NZ	LYS	B	154	43.445	39.657	-7.416	1.00	20.51
ATOM	2947	C	LYS	B	154	39.965	46.084	-7.614	1.00	15.97
ATOM	2948	O	LYS	B	154	40.506	47.199	-7.680	1.00	12.31
ATOM	2949	N	LEU	B	155	38.884	45.837	-6.880	1.00	14.81
ATOM	2950	CA	LEU	B	155	38.377	46.794	-5.908	1.00	14.24
ATOM	2951	CB	LEU	B	155	36.856	46.699	-5.789	1.00	12.61
ATOM	2952	CG	LEU	B	155	36.196	47.636	-4.775	1.00	11.77
ATOM	2953	CD1	LEU	B	155	36.154	49.071	-5.302	1.00	11.09
ATOM	2954	CD2	LEU	B	155	34.808	47.145	-4.401	1.00	11.76
ATOM	2955	C	LEU	B	155	39.041	46.564	-4.548	1.00	14.26
ATOM	2956	O	LEU	B	155	39.190	45.419	-4.101	1.00	10.85
ATOM	2957	N	LEU	B	156	39.438	47.670	-3.915	1.00	15.80
ATOM	2958	CA	LEU	B	156	40.138	47.663	-2.629	1.00	18.23
ATOM	2959	CB	LEU	B	156	41.414	48.506	-2.701	1.00	17.38
ATOM	2960	CG	LEU	B	156	42.311	48.370	-3.926	1.00	17.09
ATOM	2961	CD1	LEU	B	156	42.840	49.740	-4.332	1.00	16.63
ATOM	2962	CD2	LEU	B	156	43.448	47.393	-3.654	1.00	17.25
ATOM	2963	C	LEU	B	156	39.261	48.172	-1.482	1.00	20.43
ATOM	2964	O	LEU	B	156	39.554	47.921	-0.304	1.00	21.20
ATOM	2965	N	GLY	B	157	38.198	48.893	-1.826	1.00	20.49
ATOM	2966	CA	GLY	B	157	37.266	49.365	-0.830	1.00	24.58
ATOM	2967	C	GLY	B	157	36.560	50.620	-1.251	1.00	28.95
ATOM	2968	O	GLY	B	157	37.093	51.391	-2.042	1.00	29.72
ATOM	2969	N	LYS	B	158	35.353	50.808	-0.723	1.00	34.92
ATOM	2970	CA	LYS	B	158	34.592	52.039	-0.929	1.00	40.31
ATOM	2971	CB	LYS	B	158	33.322	51.795	-1.769	1.00	39.42
ATOM	2972	CG	LYS	B	158	32.725	50.392	-1.706	1.00	40.69
ATOM	2973	CD	LYS	B	158	31.565	50.256	-2.706	1.00	42.09
ATOM	2974	CE	LYS	B	158	30.898	48.879	-2.649	1.00	41.38
ATOM	2975	NZ	LYS	B	158	29.410	48.973	-2.590	1.00	39.96
ATOM	2976	C	LYS	B	158	34.254	52.772	0.383	1.00	44.49
ATOM	2977	O	LYS	B	158	34.478	52.258	1.490	1.00	45.65
ATOM	2978	N	GLY	B	159	33.746	53.993	0.225	1.00	47.89
ATOM	2979	CA	GLY	B	159	33.221	54.813	1.307	1.00	49.52
ATOM	2980	C	GLY	B	159	32.291	55.862	0.710	1.00	51.26
ATOM	2981	O	GLY	B	159	32.573	56.400	-0.372	1.00	53.43
ATOM	2982	N	THR	B	160	31.193	56.145	1.416	1.00	50.37
ATOM	2983	CA	THR	B	160	30.089	57.021	0.961	1.00	49.09
ATOM	2984	CB	THR	B	160	29.831	58.176	1.987	1.00	49.54
ATOM	2985	OG1	THR	B	160	30.600	57.960	3.181	1.00	49.35
ATOM	2986	CG2	THR	B	160	28.381	58.146	2.489	1.00	48.18
ATOM	2987	C	THR	B	160	30.108	57.566	-0.491	1.00	47.74
ATOM	2988	O	THR	B	160	29.157	57.354	-1.244	1.00	46.68
ATOM	2989	N	PHE	B	161	31.181	58.256	-0.874	1.00	47.18
ATOM	2990	CA	PHE	B	161	31.228	58.982	-2.147	1.00	47.38
ATOM	2991	CB	PHE	B	161	32.199	60.165	-2.050	1.00	50.56
ATOM	2992	CG	PHE	B	161	31.926	61.076	-0.881	1.00	53.82
ATOM	2993	CD1	PHE	B	161	32.666	60.957	0.300	1.00	55.99

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	2994	CE1	PHE	B	161	32.418	61.794	1.395	1.00	56.48
ATOM	2995	CZ	PHE	B	161	31.414	62.757	1.310	1.00	56.78
ATOM	2996	CE2	PHE	B	161	30.663	62.881	0.131	1.00	55.40
ATOM	2997	CD2	PHE	B	161	30.923	62.042	-0.953	1.00	54.09
ATOM	2998	C	PHE	B	161	31.555	58.123	-3.367	1.00	44.90
ATOM	2999	O	PHE	B	161	30.964	58.309	-4.436	1.00	42.47
ATOM	3000	N	GLY	B	162	32.498	57.195	-3.204	1.00	43.68
ATOM	3001	CA	GLY	B	162	32.929	56.332	-4.295	1.00	40.50
ATOM	3002	C	GLY	B	162	33.958	55.267	-3.933	1.00	37.19
ATOM	3003	O	GLY	B	162	34.288	55.058	-2.756	1.00	38.92
ATOM	3004	N	LYS	B	163	34.485	54.614	-4.966	1.00	30.26
ATOM	3005	CA	LYS	B	163	35.339	53.436	-4.811	1.00	24.46
ATOM	3006	CB	LYS	B	163	35.023	52.437	-5.931	1.00	25.68
ATOM	3007	CG	LYS	B	163	33.544	52.038	-6.035	1.00	26.84
ATOM	3008	CD	LYS	B	163	32.951	52.293	-7.428	1.00	25.06
ATOM	3009	CE	LYS	B	163	31.425	52.207	-7.399	1.00	23.84
ATOM	3010	NZ	LYS	B	163	30.861	51.757	-8.698	1.00	22.80
ATOM	3011	C	LYS	B	163	36.844	53.752	-4.786	1.00	19.56
ATOM	3012	O	LYS	B	163	37.265	54.860	-5.119	1.00	16.54
ATOM	3013	N	VAL	B	164	37.648	52.776	-4.370	1.00	15.92
ATOM	3014	CA	VAL	B	164	39.100	52.863	-4.506	1.00	15.88
ATOM	3015	CB	VAL	B	164	39.838	53.061	-3.150	1.00	19.18
ATOM	3016	CG1	VAL	B	164	41.352	53.009	-3.331	1.00	19.31
ATOM	3017	CG2	VAL	B	164	39.460	54.385	-2.512	1.00	21.61
ATOM	3018	C	VAL	B	164	39.580	51.598	-5.196	1.00	14.60
ATOM	3019	O	VAL	B	164	39.533	50.511	-4.621	1.00	11.90
ATOM	3020	N	ILE	B	165	40.037	51.763	-6.437	1.00	16.31
ATOM	3021	CA	ILE	B	165	40.376	50.649	-7.324	1.00	14.66
ATOM	3022	CB	ILE	B	165	39.550	50.745	-8.627	1.00	12.90
ATOM	3023	CG1	ILE	B	165	38.107	50.325	-8.357	1.00	12.23
ATOM	3024	CD1	ILE	B	165	37.081	51.296	-8.886	1.00	11.23
ATOM	3025	CG2	ILE	B	165	40.161	49.897	-9.746	1.00	11.95
ATOM	3026	C	ILE	B	165	41.868	50.588	-7.640	1.00	15.08
ATOM	3027	O	ILE	B	165	42.523	51.627	-7.837	1.00	12.74
ATOM	3028	N	LEU	B	166	42.387	49.358	-7.676	1.00	14.35
ATOM	3029	CA	LEU	B	166	43.763	49.103	-8.079	1.00	13.67
ATOM	3030	CB	LEU	B	166	44.236	47.727	-7.608	1.00	12.75
ATOM	3031	CG	LEU	B	166	45.637	47.253	-8.014	1.00	11.73
ATOM	3032	CD1	LEU	B	166	46.682	48.340	-7.858	1.00	10.66
ATOM	3033	CD2	LEU	B	166	46.023	46.052	-7.182	1.00	12.31
ATOM	3034	C	LEU	B	166	43.846	49.197	-9.586	1.00	13.54
ATOM	3035	O	LEU	B	166	43.140	48.483	-10.305	1.00	12.39
ATOM	3036	N	VAL	B	167	44.710	50.096	-10.044	1.00	13.67
ATOM	3037	CA	VAL	B	167	44.867	50.381	-11.464	1.00	14.12
ATOM	3038	CB	VAL	B	167	44.504	51.858	-11.806	1.00	15.23
ATOM	3039	CG1	VAL	B	167	43.017	52.096	-11.623	1.00	16.85
ATOM	3040	CG2	VAL	B	167	45.304	52.850	-10.965	1.00	14.24
ATOM	3041	C	VAL	B	167	46.275	50.051	-11.949	1.00	13.34
ATOM	3042	O	VAL	B	167	47.185	49.820	-11.155	1.00	13.13
ATOM	3043	N	LYS	B	168	46.444	50.015	-13.260	1.00	12.42
ATOM	3044	CA	LYS	B	168	47.757	49.823	-13.833	1.00	14.47
ATOM	3045	CB	LYS	B	168	47.987	48.347	-14.181	1.00	14.07

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3046	CG	LYS	B	168	49.353	48.034	-14.789	1.00	13.75
ATOM	3047	CD	LYS	B	168	49.213	47.397	-16.173	1.00	13.02
ATOM	3048	CE	LYS	B	168	50.510	46.765	-16.644	1.00	12.06
ATOM	3049	NZ	LYS	B	168	50.951	45.675	-15.728	1.00	11.53
ATOM	3050	C	LYS	B	168	47.871	50.714	-15.058	1.00	17.72
ATOM	3051	O	LYS	B	168	47.286	50.424	-16.108	1.00	20.51
ATOM	3052	N	GLU	B	169	48.600	51.817	-14.911	1.00	18.76
ATOM	3053	CA	GLU	B	169	48.909	52.694	-16.037	1.00	18.96
ATOM	3054	CB	GLU	B	169	49.931	53.757	-15.609	1.00	19.22
ATOM	3055	CG	GLU	B	169	49.482	55.199	-15.808	1.00	19.70
ATOM	3056	CD	GLU	B	169	50.398	55.991	-16.729	1.00	19.27
ATOM	3057	OE1	GLU	B	169	51.433	56.495	-16.242	1.00	20.27
ATOM	3058	OE2	GLU	B	169	50.079	56.118	-17.933	1.00	16.81
ATOM	3059	C	GLU	B	169	49.451	51.851	-17.202	1.00	18.66
ATOM	3060	O	GLU	B	169	50.395	51.078	-17.027	1.00	20.15
ATOM	3061	N	LYS	B	170	48.833	51.966	-18.376	1.00	17.08
ATOM	3062	CA	LYS	B	170	49.329	51.257	-19.556	1.00	13.85
ATOM	3063	CB	LYS	B	170	48.256	51.153	-20.642	1.00	10.29
ATOM	3064	CG	LYS	B	170	47.578	49.788	-20.689	1.00	7.02
ATOM	3065	CD	LYS	B	170	46.286	49.817	-21.489	1.00	4.66
ATOM	3066	CE	LYS	B	170	45.100	50.230	-20.636	1.00	2.49
ATOM	3067	NZ	LYS	B	170	44.443	51.441	-21.193	1.00	2.00
ATOM	3068	C	LYS	B	170	50.599	51.915	-20.088	1.00	14.36
ATOM	3069	O	LYS	B	170	51.599	51.236	-20.302	1.00	13.75
ATOM	3070	N	ALA	B	171	50.558	53.239	-20.255	1.00	16.89
ATOM	3071	CA	ALA	B	171	51.691	54.032	-20.757	1.00	19.89
ATOM	3072	CB	ALA	B	171	51.303	55.515	-20.861	1.00	19.72
ATOM	3073	C	ALA	B	171	53.013	53.870	-19.978	1.00	21.78
ATOM	3074	O	ALA	B	171	54.096	54.010	-20.558	1.00	20.72
ATOM	3075	N	THR	B	172	52.926	53.591	-18.676	1.00	24.55
ATOM	3076	CA	THR	B	172	54.122	53.310	-17.868	1.00	26.35
ATOM	3077	CB	THR	B	172	54.290	54.312	-16.669	1.00	26.26
ATOM	3078	OG1	THR	B	172	53.073	54.406	-15.920	1.00	26.87
ATOM	3079	CG2	THR	B	172	54.537	55.747	-17.156	1.00	25.39
ATOM	3080	C	THR	B	172	54.205	51.851	-17.383	1.00	27.04
ATOM	3081	O	THR	B	172	55.265	51.403	-16.944	1.00	27.20
ATOM	3082	N	GLY	B	173	53.096	51.116	-17.469	1.00	27.89
ATOM	3083	CA	GLY	B	173	53.049	49.732	-17.017	1.00	29.84
ATOM	3084	C	GLY	B	173	53.130	49.562	-15.504	1.00	32.31
ATOM	3085	O	GLY	B	173	53.339	48.447	-15.015	1.00	33.58
ATOM	3086	N	ARG	B	174	52.965	50.662	-14.765	1.00	32.20
ATOM	3087	CA	ARG	B	174	53.067	50.655	-13.306	1.00	31.81
ATOM	3088	CB	ARG	B	174	53.850	51.879	-12.818	1.00	32.79
ATOM	3089	CG	ARG	B	174	55.361	51.729	-12.926	1.00	33.41
ATOM	3090	CD	ARG	B	174	56.140	52.267	-11.729	1.00	33.86
ATOM	3091	NE	ARG	B	174	57.584	52.129	-11.922	1.00	33.77
ATOM	3092	CZ	ARG	B	174	58.389	53.082	-12.393	1.00	33.88
ATOM	3093	NH1	ARG	B	174	57.913	54.281	-12.729	1.00	32.54
ATOM	3094	NH2	ARG	B	174	59.684	52.833	-12.532	1.00	34.39
ATOM	3095	C	ARG	B	174	51.688	50.596	-12.648	1.00	31.62
ATOM	3096	O	ARG	B	174	50.675	50.833	-13.309	1.00	31.31
ATOM	3097	N	TYR	B	175	51.661	50.281	-11.350	1.00	30.75

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3098	CA	TYR	B	175	50.414	50.076	-10.609	1.00	28.48
ATOM	3099	CB	TYR	B	175	50.467	48.755	-9.834	1.00	28.93
ATOM	3100	CG	TYR	B	175	50.536	47.515	-10.703	1.00	30.55
ATOM	3101	CD1	TYR	B	175	51.766	46.953	-11.057	1.00	31.60
ATOM	3102	CE1	TYR	B	175	51.837	45.808	-11.863	1.00	32.41
ATOM	3103	CZ	TYR	B	175	50.666	45.215	-12.318	1.00	32.43
ATOM	3104	OH	TYR	B	175	50.731	44.088	-13.108	1.00	31.58
ATOM	3105	CE2	TYR	B	175	49.431	45.754	-11.976	1.00	32.14
ATOM	3106	CD2	TYR	B	175	49.373	46.898	-11.170	1.00	31.36
ATOM	3107	C	TYR	B	175	50.160	51.219	-9.638	1.00	27.23
ATOM	3108	O	TYR	B	175	51.102	51.746	-9.058	1.00	29.24
ATOM	3109	N	TYR	B	176	48.892	51.601	-9.471	1.00	26.33
ATOM	3110	CA	TYR	B	176	48.479	52.591	-8.456	1.00	24.31
ATOM	3111	CB	TYR	B	176	48.531	54.021	-9.008	1.00	25.59
ATOM	3112	CG	TYR	B	176	49.875	54.435	-9.556	1.00	26.87
ATOM	3113	CD1	TYR	B	176	50.141	54.351	-10.922	1.00	27.53
ATOM	3114	CE1	TYR	B	176	51.373	54.726	-11.440	1.00	29.97
ATOM	3115	CZ	TYR	B	176	52.364	55.192	-10.586	1.00	30.78
ATOM	3116	OH	TYR	B	176	53.588	55.564	-11.109	1.00	30.86
ATOM	3117	CE2	TYR	B	176	52.122	55.283	-9.216	1.00	29.84
ATOM	3118	CD2	TYR	B	176	50.881	54.904	-8.712	1.00	27.21
ATOM	3119	C	TYR	B	176	47.085	52.330	-7.873	1.00	21.31
ATOM	3120	O	TYR	B	176	46.367	51.428	-8.305	1.00	19.62
ATOM	3121	N	ALA	B	177	46.716	53.125	-6.877	1.00	19.77
ATOM	3122	CA	ALA	B	177	45.393	53.031	-6.273	1.00	18.79
ATOM	3123	CB	ALA	B	177	45.492	53.020	-4.750	1.00	17.23
ATOM	3124	C	ALA	B	177	44.578	54.216	-6.745	1.00	16.22
ATOM	3125	O	ALA	B	177	45.040	55.356	-6.657	1.00	16.95
ATOM	3126	N	MET	B	178	43.381	53.958	-7.264	1.00	11.19
ATOM	3127	CA	MET	B	178	42.548	55.053	-7.727	1.00	8.24
ATOM	3128	CB	MET	B	178	42.176	54.904	-9.194	1.00	10.55
ATOM	3129	CG	MET	B	178	41.649	56.199	-9.816	1.00	9.81
ATOM	3130	SD	MET	B	178	41.668	56.172	-11.623	1.00	10.61
ATOM	3131	CE	MET	B	178	40.404	54.917	-11.993	1.00	8.01
ATOM	3132	C	MET	B	178	41.304	55.236	-6.904	1.00	6.62
ATOM	3133	O	MET	B	178	40.388	54.420	-6.948	1.00	5.81
ATOM	3134	N	LYS	B	179	41.290	56.325	-6.149	1.00	6.16
ATOM	3135	CA	LYS	B	179	40.093	56.777	-5.478	1.00	5.71
ATOM	3136	CB	LYS	B	179	40.448	57.681	-4.294	1.00	8.85
ATOM	3137	CG	LYS	B	179	39.254	58.071	-3.420	1.00	11.61
ATOM	3138	CD	LYS	B	179	39.664	58.954	-2.245	1.00	13.48
ATOM	3139	CE	LYS	B	179	38.491	59.218	-1.302	1.00	13.08
ATOM	3140	NZ	LYS	B	179	38.953	59.602	0.065	1.00	12.82
ATOM	3141	C	LYS	B	179	39.293	57.535	-6.518	1.00	4.26
ATOM	3142	O	LYS	B	179	39.775	58.508	-7.095	1.00	5.59
ATOM	3143	N	ILE	B	180	38.084	57.055	-6.775	1.00	3.99
ATOM	3144	CA	ILE	B	180	37.161	57.669	-7.726	1.00	3.85
ATOM	3145	CB	ILE	B	180	36.579	56.590	-8.694	1.00	2.03
ATOM	3146	CG1	ILE	B	180	37.665	56.013	-9.598	1.00	2.00
ATOM	3147	CD1	ILE	B	180	38.046	54.594	-9.232	1.00	2.00
ATOM	3148	CG2	ILE	B	180	35.413	57.119	-9.517	1.00	2.00
ATOM	3149	C	ILE	B	180	36.043	58.293	-6.909	1.00	6.25

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3150	O	ILE	B	180	35.517	57.678	-5.974	1.00	5.92
ATOM	3151	N	LEU	B	181	35.681	59.519	-7.246	1.00	8.25
ATOM	3152	CA	LEU	B	181	34.531	60.137	-6.614	1.00	12.38
ATOM	3153	CB	LEU	B	181	34.945	61.375	-5.821	1.00	11.67
ATOM	3154	CG	LEU	B	181	36.354	61.423	-5.230	1.00	12.56
ATOM	3155	CD1	LEU	B	181	36.761	62.852	-4.962	1.00	13.98
ATOM	3156	CD2	LEU	B	181	36.437	60.607	-3.958	1.00	14.82
ATOM	3157	C	LEU	B	181	33.543	60.506	-7.700	1.00	15.82
ATOM	3158	O	LEU	B	181	33.953	60.842	-8.811	1.00	16.82
ATOM	3159	N	LYS	B	182	32.250	60.413	-7.390	1.00	17.80
ATOM	3160	CA	LYS	B	182	31.205	60.888	-8.294	1.00	18.83
ATOM	3161	CB	LYS	B	182	29.913	60.081	-8.123	1.00	20.70
ATOM	3162	CG	LYS	B	182	29.485	59.293	-9.361	1.00	22.58
ATOM	3163	CD	LYS	B	182	28.383	58.287	-9.032	1.00	24.37
ATOM	3164	CE	LYS	B	182	28.941	57.022	-8.378	1.00	24.69
ATOM	3165	NZ	LYS	B	182	29.450	56.050	-9.388	1.00	26.49
ATOM	3166	C	LYS	B	182	30.959	62.368	-8.016	1.00	18.52
ATOM	3167	O	LYS	B	182	30.591	62.751	-6.901	1.00	18.92
ATOM	3168	N	LYS	B	183	31.176	63.198	-9.032	1.00	17.38
ATOM	3169	CA	LYS	B	183	31.010	64.640	-8.894	1.00	16.72
ATOM	3170	CB	LYS	B	183	31.362	65.342	-10.208	1.00	16.79
ATOM	3171	CG	LYS	B	183	32.870	65.489	-10.445	1.00	16.98
ATOM	3172	CD	LYS	B	183	33.218	65.631	-11.923	1.00	16.75
ATOM	3173	CE	LYS	B	183	33.622	67.058	-12.288	1.00	16.29
ATOM	3174	NZ	LYS	B	183	33.600	67.290	-13.766	1.00	15.14
ATOM	3175	C	LYS	B	183	29.596	64.991	-8.429	1.00	16.79
ATOM	3176	O	LYS	B	183	29.403	65.932	-7.658	1.00	16.80
ATOM	3177	N	GLU	B	184	28.624	64.205	-8.890	1.00	18.36
ATOM	3178	CA	GLU	B	184	27.229	64.303	-8.467	1.00	20.14
ATOM	3179	CB	GLU	B	184	26.403	63.186	-9.124	1.00	21.73
ATOM	3180	CG	GLU	B	184	24.893	63.312	-8.959	1.00	23.96
ATOM	3181	CD	GLU	B	184	24.176	63.631	-10.265	1.00	26.46
ATOM	3182	OE1	GLU	B	184	22.961	63.935	-10.221	1.00	27.52
ATOM	3183	OE2	GLU	B	184	24.816	63.582	-11.339	1.00	26.92
ATOM	3184	C	GLU	B	184	27.099	64.224	-6.945	1.00	20.17
ATOM	3185	O	GLU	B	184	26.534	65.124	-6.316	1.00	21.28
ATOM	3186	N	VAL	B	185	27.638	63.152	-6.367	1.00	18.26
ATOM	3187	CA	VAL	B	185	27.503	62.880	-4.938	1.00	17.96
ATOM	3188	CB	VAL	B	185	28.036	61.455	-4.556	1.00	20.09
ATOM	3189	CG1	VAL	B	185	27.886	61.172	-3.051	1.00	19.56
ATOM	3190	CG2	VAL	B	185	27.334	60.367	-5.373	1.00	19.88
ATOM	3191	C	VAL	B	185	28.173	63.970	-4.097	1.00	15.76
ATOM	3192	O	VAL	B	185	27.611	64.411	-3.089	1.00	16.87
ATOM	3193	N	ILE	B	186	29.354	64.417	-4.520	1.00	11.10
ATOM	3194	CA	ILE	B	186	30.087	65.428	-3.770	1.00	7.49
ATOM	3195	CB	ILE	B	186	31.469	65.690	-4.396	1.00	6.65
ATOM	3196	CG1	ILE	B	186	32.498	64.768	-3.763	1.00	6.43
ATOM	3197	CD1	ILE	B	186	33.450	64.209	-4.755	1.00	8.66
ATOM	3198	CG2	ILE	B	186	31.930	67.127	-4.195	1.00	6.46
ATOM	3199	C	ILE	B	186	29.249	66.685	-3.669	1.00	6.95
ATOM	3200	O	ILE	B	186	29.222	67.338	-2.630	1.00	6.39
ATOM	3201	N	VAL	B	187	28.538	66.997	-4.744	1.00	7.91

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3202	CA	VAL	B	187	27.676	68.166	-4.767	1.00	11.34
ATOM	3203	CB	VAL	B	187	27.341	68.583	-6.221	1.00	11.96
ATOM	3204	CG1	VAL	B	187	26.043	69.397	-6.295	1.00	12.18
ATOM	3205	CG2	VAL	B	187	28.505	69.365	-6.820	1.00	11.81
ATOM	3206	C	VAL	B	187	26.420	67.910	-3.936	1.00	12.90
ATOM	3207	O	VAL	B	187	26.027	68.753	-3.123	1.00	12.41
ATOM	3208	N	ALA	B	188	25.820	66.736	-4.131	1.00	15.25
ATOM	3209	CA	ALA	B	188	24.571	66.366	-3.465	1.00	17.66
ATOM	3210	CB	ALA	B	188	24.034	65.041	-4.010	1.00	17.54
ATOM	3211	C	ALA	B	188	24.713	66.313	-1.947	1.00	19.31
ATOM	3212	O	ALA	B	188	23.905	66.903	-1.238	1.00	20.34
ATOM	3213	N	LYS	B	189	25.738	65.616	-1.456	1.00	21.45
ATOM	3214	CA	LYS	B	189	26.007	65.556	-0.018	1.00	24.50
ATOM	3215	CB	LYS	B	189	26.655	64.216	0.380	1.00	26.28
ATOM	3216	CG	LYS	B	189	26.008	63.531	1.607	1.00	28.54
ATOM	3217	CD	LYS	B	189	26.634	63.998	2.932	1.00	30.44
ATOM	3218	CE	LYS	B	189	25.610	64.074	4.068	1.00	31.09
ATOM	3219	NZ	LYS	B	189	26.298	64.060	5.396	1.00	32.57
ATOM	3220	C	LYS	B	189	26.841	66.754	0.466	1.00	25.18
ATOM	3221	O	LYS	B	189	27.235	66.821	1.640	1.00	27.28
ATOM	3222	N	ASP	B	190	27.104	67.692	-0.448	1.00	23.16
ATOM	3223	CA	ASP	B	190	27.708	68.991	-0.127	1.00	21.54
ATOM	3224	CB	ASP	B	190	26.884	69.711	0.950	1.00	21.28
ATOM	3225	CG	ASP	B	190	27.256	71.172	1.094	1.00	22.63
ATOM	3226	OD1	ASP	B	190	27.936	71.512	2.083	1.00	23.67
ATOM	3227	OD2	ASP	B	190	26.919	72.054	0.274	1.00	23.72
ATOM	3228	C	ASP	B	190	29.203	68.981	0.245	1.00	21.17
ATOM	3229	O	ASP	B	190	29.801	70.043	0.430	1.00	20.90
ATOM	3230	N	GLU	B	191	29.812	67.800	0.329	1.00	22.04
ATOM	3231	CA	GLU	B	191	31.225	67.698	0.720	1.00	23.15
ATOM	3232	CB	GLU	B	191	31.563	66.296	1.262	1.00	26.18
ATOM	3233	CG	GLU	B	191	31.707	66.218	2.784	1.00	29.43
ATOM	3234	CD	GLU	B	191	30.753	67.155	3.523	1.00	32.38
ATOM	3235	OE1	GLU	B	191	31.238	68.167	4.088	1.00	32.81
ATOM	3236	OE2	GLU	B	191	29.519	66.889	3.530	1.00	32.22
ATOM	3237	C	GLU	B	191	32.168	68.112	-0.405	1.00	20.16
ATOM	3238	O	GLU	B	191	32.860	67.284	-0.998	1.00	20.39
ATOM	3239	N	VAL	B	192	32.200	69.413	-0.667	1.00	17.94
ATOM	3240	CA	VAL	B	192	32.862	69.946	-1.846	1.00	17.27
ATOM	3241	CB	VAL	B	192	31.997	71.017	-2.545	1.00	17.63
ATOM	3242	CG1	VAL	B	192	32.745	71.618	-3.720	1.00	17.42
ATOM	3243	CG2	VAL	B	192	30.661	70.434	-2.994	1.00	16.82
ATOM	3244	C	VAL	B	192	34.209	70.546	-1.497	1.00	16.16
ATOM	3245	O	VAL	B	192	35.208	70.240	-2.150	1.00	16.58
ATOM	3246	N	ALA	B	193	34.225	71.407	-0.481	1.00	14.30
ATOM	3247	CA	ALA	B	193	35.441	72.107	-0.073	1.00	13.95
ATOM	3248	CB	ALA	B	193	35.112	73.211	0.922	1.00	12.65
ATOM	3249	C	ALA	B	193	36.506	71.156	0.490	1.00	14.42
ATOM	3250	O	ALA	B	193	37.708	71.389	0.321	1.00	13.33
ATOM	3251	N	HIS	B	194	36.050	70.087	1.147	1.00	16.49
ATOM	3252	CA	HIS	B	194	36.920	69.046	1.710	1.00	16.55
ATOM	3253	CB	HIS	B	194	36.127	68.098	2.625	1.00	16.77

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3254	CG	HIS	B	194	35.531	68.758	3.826	1.00	15.93
ATOM	3255	ND1	HIS	B	194	34.179	68.728	4.091	1.00	15.23
ATOM	3256	CE1	HIS	B	194	33.941	69.395	5.206	1.00	18.34
ATOM	3257	NE2	HIS	B	194	35.090	69.844	5.681	1.00	18.34
ATOM	3258	CD2	HIS	B	194	36.101	69.457	4.836	1.00	17.07
ATOM	3259	C	HIS	B	194	37.556	68.221	0.599	1.00	15.40
ATOM	3260	O	HIS	B	194	38.731	67.853	0.674	1.00	15.53
ATOM	3261	N	THR	B	195	36.751	67.918	-0.416	1.00	13.68
ATOM	3262	CA	THR	B	195	37.193	67.183	-1.591	1.00	12.68
ATOM	3263	CB	THR	B	195	35.980	66.953	-2.538	1.00	9.64
ATOM	3264	OG1	THR	B	195	35.635	65.563	-2.545	1.00	4.08
ATOM	3265	CG2	THR	B	195	36.321	67.239	-3.986	1.00	10.67
ATOM	3266	C	THR	B	195	38.369	67.914	-2.267	1.00	14.58
ATOM	3267	O	THR	B	195	39.315	67.278	-2.755	1.00	16.73
ATOM	3268	N	LEU	B	196	38.318	69.246	-2.258	1.00	13.55
ATOM	3269	CA	LEU	B	196	39.424	70.067	-2.741	1.00	12.15
ATOM	3270	CB	LEU	B	196	38.976	71.504	-3.002	1.00	12.80
ATOM	3271	CG	LEU	B	196	38.218	71.782	-4.293	1.00	11.62
ATOM	3272	CD1	LEU	B	196	37.301	72.963	-4.054	1.00	11.32
ATOM	3273	CD2	LEU	B	196	39.178	72.046	-5.453	1.00	12.64
ATOM	3274	C	LEU	B	196	40.556	70.064	-1.731	1.00	10.37
ATOM	3275	O	LEU	B	196	41.690	69.735	-2.080	1.00	11.36
ATOM	3276	N	THR	B	197	40.242	70.434	-0.488	1.00	8.25
ATOM	3277	CA	THR	B	197	41.204	70.393	0.612	1.00	6.50
ATOM	3278	CB	THR	B	197	40.490	70.438	1.983	1.00	7.68
ATOM	3279	OG1	THR	B	197	39.753	71.659	2.114	1.00	10.07
ATOM	3280	CG2	THR	B	197	41.496	70.549	3.093	1.00	8.76
ATOM	3281	C	THR	B	197	42.036	69.130	0.502	1.00	4.18
ATOM	3282	O	THR	B	197	43.247	69.180	0.646	1.00	2.00
ATOM	3283	N	GLU	B	198	41.372	68.009	0.224	1.00	7.75
ATOM	3284	CA	GLU	B	198	42.038	66.727	0.007	1.00	13.36
ATOM	3285	CB	GLU	B	198	41.025	65.618	-0.297	1.00	17.07
ATOM	3286	CG	GLU	B	198	41.572	64.208	-0.078	1.00	22.09
ATOM	3287	CD	GLU	B	198	40.549	63.102	-0.327	1.00	25.19
ATOM	3288	OE1	GLU	B	198	39.496	63.362	-0.966	1.00	26.00
ATOM	3289	OE2	GLU	B	198	40.807	61.956	0.118	1.00	26.31
ATOM	3290	C	GLU	B	198	43.080	66.822	-1.102	1.00	15.54
ATOM	3291	O	GLU	B	198	44.284	66.737	-0.834	1.00	16.05
ATOM	3292	N	ASN	B	199	42.617	67.011	-2.339	1.00	17.68
ATOM	3293	CA	ASN	B	199	43.513	67.213	-3.475	1.00	17.06
ATOM	3294	CB	ASN	B	199	42.756	67.766	-4.677	1.00	19.03
ATOM	3295	CG	ASN	B	199	43.647	67.937	-5.894	1.00	21.41
ATOM	3296	OD1	ASN	B	199	43.935	69.056	-6.315	1.00	23.88
ATOM	3297	ND2	ASN	B	199	44.098	66.825	-6.459	1.00	21.67
ATOM	3298	C	ASN	B	199	44.697	68.120	-3.142	1.00	15.66
ATOM	3299	O	ASN	B	199	45.836	67.751	-3.384	1.00	16.09
ATOM	3300	N	ARG	B	200	44.416	69.290	-2.573	1.00	13.84
ATOM	3301	CA	ARG	B	200	45.449	70.221	-2.128	1.00	13.10
ATOM	3302	CB	ARG	B	200	44.806	71.410	-1.417	1.00	13.13
ATOM	3303	CG	ARG	B	200	45.640	72.669	-1.415	1.00	14.66
ATOM	3304	CD	ARG	B	200	44.979	73.840	-2.118	1.00	17.08
ATOM	3305	NE	ARG	B	200	44.169	74.657	-1.214	1.00	19.01

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3306	CZ	ARG	B	200	42.902	74.407	-0.882	1.00	20.18
ATOM	3307	NH1	ARG	B	200	42.268	75.226	-0.054	1.00	21.81
ATOM	3308	NH2	ARG	B	200	42.262	73.348	-1.364	1.00	19.24
ATOM	3309	C	ARG	B	200	46.519	69.568	-1.228	1.00	13.83
ATOM	3310	O	ARG	B	200	47.717	69.638	-1.536	1.00	17.02
ATOM	3311	N	VAL	B	201	46.097	68.939	-0.130	1.00	9.96
ATOM	3312	CA	VAL	B	201	47.046	68.292	0.777	1.00	5.98
ATOM	3313	CB	VAL	B	201	46.367	67.724	2.055	1.00	2.72
ATOM	3314	CG1	VAL	B	201	47.366	66.966	2.922	1.00	2.00
ATOM	3315	CG2	VAL	B	201	45.733	68.834	2.858	1.00	2.00
ATOM	3316	C	VAL	B	201	47.765	67.202	-0.005	1.00	7.60
ATOM	3317	O	VAL	B	201	48.992	67.206	-0.090	1.00	7.95
ATOM	3318	N	LEU	B	202	46.986	66.312	-0.615	1.00	8.97
ATOM	3319	CA	LEU	B	202	47.499	65.235	-1.462	1.00	13.56
ATOM	3320	CB	LEU	B	202	46.370	64.640	-2.306	1.00	10.35
ATOM	3321	CG	LEU	B	202	45.740	63.337	-1.826	1.00	9.87
ATOM	3322	CD1	LEU	B	202	44.575	62.972	-2.723	1.00	8.92
ATOM	3323	CD2	LEU	B	202	46.749	62.196	-1.777	1.00	10.04
ATOM	3324	C	LEU	B	202	48.697	65.591	-2.376	1.00	19.28
ATOM	3325	O	LEU	B	202	49.604	64.765	-2.548	1.00	22.90
ATOM	3326	N	GLN	B	203	48.705	66.789	-2.970	1.00	20.31
ATOM	3327	CA	GLN	B	203	49.865	67.208	-3.766	1.00	20.11
ATOM	3328	CB	GLN	B	203	49.501	67.955	-5.069	1.00	20.67
ATOM	3329	CG	GLN	B	203	48.030	68.019	-5.470	1.00	19.67
ATOM	3330	CD	GLN	B	203	47.634	69.363	-6.095	1.00	18.61
ATOM	3331	OE1	GLN	B	203	48.314	70.379	-5.909	1.00	17.21
ATOM	3332	NE2	GLN	B	203	46.527	69.364	-6.827	1.00	18.03
ATOM	3333	C	GLN	B	203	50.879	68.021	-2.958	1.00	20.30
ATOM	3334	O	GLN	B	203	52.082	67.749	-3.007	1.00	20.81
ATOM	3335	N	ASN	B	204	50.402	69.010	-2.212	1.00	19.66
ATOM	3336	CA	ASN	B	204	51.317	69.919	-1.530	1.00	22.16
ATOM	3337	CB	ASN	B	204	50.617	71.231	-1.188	1.00	20.11
ATOM	3338	CG	ASN	B	204	50.676	72.204	-2.321	1.00	20.95
ATOM	3339	OD1	ASN	B	204	51.691	72.869	-2.525	1.00	22.09
ATOM	3340	ND2	ASN	B	204	49.600	72.276	-3.098	1.00	21.15
ATOM	3341	C	ASN	B	204	52.038	69.320	-0.314	1.00	24.57
ATOM	3342	O	ASN	B	204	52.479	70.044	0.585	1.00	27.00
ATOM	3343	N	SER	B	205	52.175	67.996	-0.308	1.00	23.83
ATOM	3344	CA	SER	B	205	52.816	67.285	0.796	1.00	22.84
ATOM	3345	CB	SER	B	205	51.768	66.650	1.720	1.00	20.77
ATOM	3346	OG	SER	B	205	50.927	67.649	2.276	1.00	18.07
ATOM	3347	C	SER	B	205	53.812	66.243	0.290	1.00	22.23
ATOM	3348	O	SER	B	205	53.831	65.905	-0.898	1.00	21.65
ATOM	3349	N	ARG	B	206	54.635	65.753	1.213	1.00	19.78
ATOM	3350	CA	ARG	B	206	55.770	64.893	0.912	1.00	17.79
ATOM	3351	CB	ARG	B	206	56.790	65.621	0.027	1.00	20.24
ATOM	3352	CG	ARG	B	206	56.739	65.227	-1.437	1.00	23.99
ATOM	3353	CD	ARG	B	206	57.007	66.375	-2.404	1.00	26.62
ATOM	3354	NE	ARG	B	206	55.770	67.008	-2.854	1.00	29.11
ATOM	3355	CZ	ARG	B	206	55.708	68.165	-3.504	1.00	31.55
ATOM	3356	NH1	ARG	B	206	54.528	68.653	-3.869	1.00	32.36
ATOM	3357	NH2	ARG	B	206	56.820	68.840	-3.793	1.00	31.99

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3358	C	ARG	B	206	56.410	64.489	2.237	1.00	13.72
ATOM	3359	O	ARG	B	206	57.137	65.259	2.866	1.00	14.06
ATOM	3360	N	HIS	B	207	56.109	63.275	2.659	1.00	7.72
ATOM	3361	CA	HIS	B	207	56.562	62.746	3.925	1.00	4.20
ATOM	3362	CB	HIS	B	207	55.678	63.286	5.052	1.00	2.00
ATOM	3363	CG	HIS	B	207	56.146	62.919	6.422	1.00	2.00
ATOM	3364	ND1	HIS	B	207	56.694	63.836	7.289	1.00	2.00
ATOM	3365	CE1	HIS	B	207	57.014	63.235	8.421	1.00	2.00
ATOM	3366	NE2	HIS	B	207	56.689	61.958	8.320	1.00	2.00
ATOM	3367	CD2	HIS	B	207	56.142	61.734	7.080	1.00	2.00
ATOM	3368	C	HIS	B	207	56.402	61.235	3.740	1.00	4.66
ATOM	3369	O	HIS	B	207	55.416	60.803	3.136	1.00	6.44
ATOM	3370	N	PRO	B	208	57.371	60.441	4.195	1.00	2.15
ATOM	3371	CA	PRO	B	208	57.394	58.998	3.909	1.00	2.00
ATOM	3372	CB	PRO	B	208	58.703	58.539	4.539	1.00	2.00
ATOM	3373	CG	PRO	B	208	59.506	59.778	4.680	1.00	2.36
ATOM	3374	CD	PRO	B	208	58.547	60.869	4.972	1.00	2.00
ATOM	3375	C	PRO	B	208	56.237	58.173	4.466	1.00	3.08
ATOM	3376	O	PRO	B	208	56.101	57.023	4.045	1.00	4.07
ATOM	3377	N	PHE	B	209	55.438	58.719	5.383	1.00	6.28
ATOM	3378	CA	PHE	B	209	54.255	57.999	5.901	1.00	9.54
ATOM	3379	CB	PHE	B	209	54.385	57.703	7.408	1.00	10.16
ATOM	3380	CG	PHE	B	209	55.790	57.367	7.832	1.00	12.18
ATOM	3381	CD1	PHE	B	209	56.473	56.298	7.248	1.00	11.99
ATOM	3382	CE1	PHE	B	209	57.772	56.003	7.611	1.00	8.61
ATOM	3383	CZ	PHE	B	209	58.403	56.773	8.564	1.00	8.44
ATOM	3384	CE2	PHE	B	209	57.746	57.840	9.148	1.00	9.66
ATOM	3385	CD2	PHE	B	209	56.448	58.140	8.777	1.00	11.74
ATOM	3386	C	PHE	B	209	52.935	58.699	5.562	1.00	10.55
ATOM	3387	O	PHE	B	209	51.904	58.450	6.173	1.00	12.81
ATOM	3388	N	LEU	B	210	53.000	59.587	4.576	1.00	10.78
ATOM	3389	CA	LEU	B	210	51.830	60.166	3.938	1.00	8.21
ATOM	3390	CB	LEU	B	210	51.943	61.695	3.914	1.00	4.33
ATOM	3391	CG	LEU	B	210	52.009	62.451	5.241	1.00	2.22
ATOM	3392	CD1	LEU	B	210	51.877	63.949	5.029	1.00	2.00
ATOM	3393	CD2	LEU	B	210	50.944	61.942	6.204	1.00	3.54
ATOM	3394	C	LEU	B	210	51.783	59.635	2.512	1.00	8.78
ATOM	3395	O	LEU	B	210	52.806	59.621	1.825	1.00	8.97
ATOM	3396	N	THR	B	211	50.610	59.195	2.062	1.00	9.14
ATOM	3397	CA	THR	B	211	50.460	58.767	0.674	1.00	9.56
ATOM	3398	CB	THR	B	211	49.028	58.304	0.376	1.00	9.73
ATOM	3399	OG1	THR	B	211	48.541	57.521	1.470	1.00	14.21
ATOM	3400	CG2	THR	B	211	49.026	57.307	-0.757	1.00	8.12
ATOM	3401	C	THR	B	211	50.846	59.903	-0.259	1.00	11.00
ATOM	3402	O	THR	B	211	50.470	61.058	-0.038	1.00	11.02
ATOM	3403	N	ALA	B	212	51.627	59.566	-1.282	1.00	12.18
ATOM	3404	CA	ALA	B	212	52.005	60.519	-2.318	1.00	12.85
ATOM	3405	CB	ALA	B	212	53.461	60.319	-2.725	1.00	12.10
ATOM	3406	C	ALA	B	212	51.078	60.402	-3.532	1.00	13.78
ATOM	3407	O	ALA	B	212	50.625	59.309	-3.887	1.00	12.07
ATOM	3408	N	LEU	B	213	50.802	61.545	-4.156	1.00	15.82
ATOM	3409	CA	LEU	B	213	49.935	61.620	-5.325	1.00	15.71

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3410	CB	LEU	B	213	49.039	62.857	-5.233	1.00	13.93
ATOM	3411	CG	LEU	B	213	47.861	63.017	-6.193	1.00	12.55
ATOM	3412	CD1	LEU	B	213	46.823	61.925	-5.995	1.00	12.37
ATOM	3413	CD2	LEU	B	213	47.242	64.382	-5.980	1.00	11.68
ATOM	3414	C	LEU	B	213	50.755	61.670	-6.605	1.00	17.99
ATOM	3415	O	LEU	B	213	51.598	62.553	-6.781	1.00	18.02
ATOM	3416	N	LYS	B	214	50.515	60.702	-7.486	1.00	20.78
ATOM	3417	CA	LYS	B	214	51.087	60.715	-8.825	1.00	20.72
ATOM	3418	CB	LYS	B	214	51.331	59.292	-9.348	1.00	20.15
ATOM	3419	CG	LYS	B	214	51.802	59.215	-10.796	1.00	20.99
ATOM	3420	CD	LYS	B	214	53.276	58.835	-10.909	1.00	22.86
ATOM	3421	CE	LYS	B	214	53.753	58.847	-12.366	1.00	22.87
ATOM	3422	NZ	LYS	B	214	55.060	59.553	-12.527	1.00	22.08
ATOM	3423	C	LYS	B	214	50.132	61.491	-9.721	1.00	21.98
ATOM	3424	O	LYS	B	214	50.454	62.602	-10.143	1.00	25.32
ATOM	3425	N	TYR	B	215	48.953	60.934	-9.987	1.00	22.06
ATOM	3426	CA	TYR	B	215	47.995	61.604	-10.865	1.00	24.71
ATOM	3427	CB	TYR	B	215	47.602	60.726	-12.070	1.00	24.65
ATOM	3428	CG	TYR	B	215	48.755	60.297	-12.968	1.00	25.07
ATOM	3429	CD1	TYR	B	215	49.532	61.235	-13.648	1.00	24.49
ATOM	3430	CE1	TYR	B	215	50.592	60.836	-14.469	1.00	24.75
ATOM	3431	CZ	TYR	B	215	50.873	59.484	-14.619	1.00	25.14
ATOM	3432	OH	TYR	B	215	51.913	59.076	-15.423	1.00	25.97
ATOM	3433	CE2	TYR	B	215	50.113	58.535	-13.961	1.00	25.56
ATOM	3434	CD2	TYR	B	215	49.058	58.944	-13.143	1.00	25.71
ATOM	3435	C	TYR	B	215	46.750	62.088	-10.130	1.00	25.72
ATOM	3436	O	TYR	B	215	46.250	61.425	-9.218	1.00	25.47
ATOM	3437	N	SER	B	216	46.278	63.263	-10.542	1.00	27.13
ATOM	3438	CA	SER	B	216	44.990	63.810	-10.127	1.00	27.09
ATOM	3439	CB	SER	B	216	45.186	64.894	-9.075	1.00	26.03
ATOM	3440	OG	SER	B	216	43.940	65.456	-8.716	1.00	26.14
ATOM	3441	C	SER	B	216	44.269	64.385	-11.350	1.00	27.91
ATOM	3442	O	SER	B	216	44.854	65.159	-12.117	1.00	31.31
ATOM	3443	N	PHE	B	217	43.006	64.004	-11.535	1.00	25.40
ATOM	3444	CA	PHE	B	217	42.244	64.414	-12.714	1.00	22.13
ATOM	3445	CB	PHE	B	217	42.733	63.662	-13.955	1.00	22.21
ATOM	3446	CG	PHE	B	217	42.442	62.190	-13.930	1.00	23.35
ATOM	3447	CD1	PHE	B	217	43.357	61.297	-13.382	1.00	23.90
ATOM	3448	CE1	PHE	B	217	43.096	59.931	-13.358	1.00	23.73
ATOM	3449	CZ	PHE	B	217	41.911	59.446	-13.887	1.00	24.33
ATOM	3450	CE2	PHE	B	217	40.986	60.331	-14.440	1.00	25.02
ATOM	3451	CD2	PHE	B	217	41.257	61.691	-14.464	1.00	23.98
ATOM	3452	C	PHE	B	217	40.743	64.213	-12.540	1.00	21.34
ATOM	3453	O	PHE	B	217	40.271	63.891	-11.450	1.00	22.92
ATOM	3454	N	GLN	B	218	40.005	64.387	-13.634	1.00	19.79
ATOM	3455	CA	GLN	B	218	38.547	64.322	-13.623	1.00	18.96
ATOM	3456	CB	GLN	B	218	37.970	65.679	-13.196	1.00	17.85
ATOM	3457	CG	GLN	B	218	38.334	66.843	-14.128	1.00	16.69
ATOM	3458	CD	GLN	B	218	38.074	68.205	-13.523	1.00	15.21
ATOM	3459	OE1	GLN	B	218	36.941	68.527	-13.161	1.00	15.00
ATOM	3460	NE2	GLN	B	218	39.119	69.017	-13.427	1.00	14.27
ATOM	3461	C	GLN	B	218	37.969	63.925	-14.988	1.00	19.16

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3462	O	GLN	B	218	38.573	64.193	-16.032	1.00	21.40
ATOM	3463	N	THR	B	219	36.806	63.278	-14.969	1.00	17.52
ATOM	3464	CA	THR	B	219	35.989	63.129	-16.171	1.00	14.96
ATOM	3465	CB	THR	B	219	35.439	61.672	-16.356	1.00	11.54
ATOM	3466	OG1	THR	B	219	34.249	61.487	-15.582	1.00	6.79
ATOM	3467	CG2	THR	B	219	36.390	60.637	-15.794	1.00	9.95
ATOM	3468	C	THR	B	219	34.859	64.155	-16.109	1.00	17.47
ATOM	3469	O	THR	B	219	34.877	65.058	-15.270	1.00	16.56
ATOM	3470	N	HIS	B	220	33.890	64.020	-17.011	1.00	22.23
ATOM	3471	CA	HIS	B	220	32.696	64.868	-17.040	1.00	24.44
ATOM	3472	CB	HIS	B	220	31.836	64.514	-18.263	1.00	23.54
ATOM	3473	CG	HIS	B	220	31.614	63.043	-18.428	1.00	24.02
ATOM	3474	ND1	HIS	B	220	32.637	62.163	-18.714	1.00	24.07
ATOM	3475	CE1	HIS	B	220	32.155	60.934	-18.774	1.00	24.52
ATOM	3476	NE2	HIS	B	220	30.856	60.986	-18.537	1.00	25.10
ATOM	3477	CD2	HIS	B	220	30.494	62.293	-18.313	1.00	24.34
ATOM	3478	C	HIS	B	220	31.878	64.754	-15.738	1.00	25.13
ATOM	3479	O	HIS	B	220	31.328	65.750	-15.264	1.00	25.10
ATOM	3480	N	ASP	B	221	31.823	63.549	-15.161	1.00	26.39
ATOM	3481	CA	ASP	B	221	31.053	63.291	-13.929	1.00	27.34
ATOM	3482	CB	ASP	B	221	29.705	62.598	-14.253	1.00	28.05
ATOM	3483	CG	ASP	B	221	29.857	61.118	-14.609	1.00	28.22
ATOM	3484	OD1	ASP	B	221	29.853	60.277	-13.684	1.00	28.41
ATOM	3485	OD2	ASP	B	221	29.964	60.702	-15.784	1.00	28.02
ATOM	3486	C	ASP	B	221	31.821	62.569	-12.784	1.00	26.18
ATOM	3487	O	ASP	B	221	31.269	62.325	-11.702	1.00	25.24
ATOM	3488	N	ARG	B	222	33.093	62.255	-13.020	1.00	24.14
ATOM	3489	CA	ARG	B	222	33.907	61.551	-12.038	1.00	22.59
ATOM	3490	CB	ARG	B	222	34.354	60.200	-12.600	1.00	22.44
ATOM	3491	CG	ARG	B	222	33.722	59.003	-11.922	1.00	23.64
ATOM	3492	CD	ARG	B	222	32.672	58.286	-12.746	1.00	23.94
ATOM	3493	NE	ARG	B	222	33.190	57.049	-13.322	1.00	25.81
ATOM	3494	CZ	ARG	B	222	33.432	56.860	-14.619	1.00	28.20
ATOM	3495	NH1	ARG	B	222	33.205	57.827	-15.505	1.00	29.58
ATOM	3496	NH2	ARG	B	222	33.905	55.694	-15.039	1.00	29.09
ATOM	3497	C	ARG	B	222	35.125	62.365	-11.604	1.00	23.12
ATOM	3498	O	ARG	B	222	35.822	62.940	-12.437	1.00	23.43
ATOM	3499	N	LEU	B	223	35.366	62.422	-10.295	1.00	23.95
ATOM	3500	CA	LEU	B	223	36.604	62.984	-9.750	1.00	22.51
ATOM	3501	CB	LEU	B	223	36.334	63.850	-8.516	1.00	21.97
ATOM	3502	CG	LEU	B	223	36.196	65.376	-8.607	1.00	22.19
ATOM	3503	CD1	LEU	B	223	36.734	66.019	-7.341	1.00	21.37
ATOM	3504	CD2	LEU	B	223	36.866	65.985	-9.832	1.00	22.54
ATOM	3505	C	LEU	B	223	37.546	61.843	-9.395	1.00	21.59
ATOM	3506	O	LEU	B	223	37.108	60.786	-8.925	1.00	18.49
ATOM	3507	N	CYS	B	224	38.839	62.063	-9.619	1.00	22.66
ATOM	3508	CA	CYS	B	224	39.822	60.995	-9.490	1.00	24.10
ATOM	3509	CB	CYS	B	224	40.166	60.425	-10.862	1.00	25.39
ATOM	3510	SG	CYS	B	224	39.348	58.863	-11.221	1.00	29.27
ATOM	3511	C	CYS	B	224	41.104	61.396	-8.784	1.00	23.67
ATOM	3512	O	CYS	B	224	41.647	62.483	-8.994	1.00	24.47
ATOM	3513	N	PHE	B	225	41.575	60.484	-7.945	1.00	22.95

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3514	CA	PHE	B	225	42.872	60.593	-7.315	1.00	21.39
ATOM	3515	CB	PHE	B	225	42.710	60.808	-5.824	1.00	22.81
ATOM	3516	CG	PHE	B	225	42.062	62.102	-5.466	1.00	23.36
ATOM	3517	CD1	PHE	B	225	40.862	62.115	-4.767	1.00	23.31
ATOM	3518	CE1	PHE	B	225	40.263	63.313	-4.415	1.00	23.94
ATOM	3519	CZ	PHE	B	225	40.866	64.513	-4.759	1.00	23.79
ATOM	3520	CE2	PHE	B	225	42.065	64.507	-5.457	1.00	23.30
ATOM	3521	CD2	PHE	B	225	42.657	63.309	-5.806	1.00	22.68
ATOM	3522	C	PHE	B	225	43.596	59.290	-7.554	1.00	20.16
ATOM	3523	O	PHE	B	225	43.082	58.214	-7.233	1.00	19.70
ATOM	3524	N	VAL	B	226	44.781	59.385	-8.141	1.00	18.07
ATOM	3525	CA	VAL	B	226	45.586	58.204	-8.397	1.00	17.13
ATOM	3526	CB	VAL	B	226	45.880	58.015	-9.896	1.00	15.53
ATOM	3527	CG1	VAL	B	226	46.529	56.668	-10.132	1.00	16.08
ATOM	3528	CG2	VAL	B	226	44.609	58.129	-10.711	1.00	13.03
ATOM	3529	C	VAL	B	226	46.875	58.304	-7.592	1.00	17.83
ATOM	3530	O	VAL	B	226	47.845	58.924	-8.027	1.00	19.87
ATOM	3531	N	MET	B	227	46.856	57.704	-6.405	1.00	17.36
ATOM	3532	CA	MET	B	227	47.985	57.740	-5.477	1.00	16.79
ATOM	3533	CB	MET	B	227	47.542	58.220	-4.087	1.00	16.52
ATOM	3534	CG	MET	B	227	46.365	57.459	-3.469	1.00	14.52
ATOM	3535	SD	MET	B	227	44.982	58.543	-3.094	1.00	11.06
ATOM	3536	CE	MET	B	227	44.157	57.589	-1.812	1.00	15.09
ATOM	3537	C	MET	B	227	48.614	56.365	-5.386	1.00	17.36
ATOM	3538	O	MET	B	227	48.024	55.384	-5.851	1.00	19.57
ATOM	3539	N	GLU	B	228	49.801	56.294	-4.788	1.00	17.38
ATOM	3540	CA	GLU	B	228	50.559	55.046	-4.732	1.00	20.06
ATOM	3541	CB	GLU	B	228	51.976	55.265	-4.177	1.00	23.13
ATOM	3542	CG	GLU	B	228	52.089	56.324	-3.092	1.00	29.42
ATOM	3543	CD	GLU	B	228	52.791	55.816	-1.840	1.00	33.76
ATOM	3544	OE1	GLU	B	228	54.034	55.938	-1.781	1.00	35.59
ATOM	3545	OE2	GLU	B	228	52.106	55.297	-0.916	1.00	35.91
ATOM	3546	C	GLU	B	228	49.814	53.958	-3.961	1.00	18.82
ATOM	3547	O	GLU	B	228	49.501	54.117	-2.787	1.00	19.18
ATOM	3548	N	TYR	B	229	49.510	52.866	-4.649	1.00	20.12
ATOM	3549	CA	TYR	B	229	48.837	51.734	-4.038	1.00	24.76
ATOM	3550	CB	TYR	B	229	48.491	50.696	-5.119	1.00	26.14
ATOM	3551	CG	TYR	B	229	48.325	49.259	-4.647	1.00	28.17
ATOM	3552	CD1	TYR	B	229	47.262	48.887	-3.821	1.00	28.49
ATOM	3553	CE1	TYR	B	229	47.111	47.566	-3.396	1.00	29.29
ATOM	3554	CZ	TYR	B	229	48.022	46.601	-3.803	1.00	28.67
ATOM	3555	OH	TYR	B	229	47.866	45.303	-3.380	1.00	29.35
ATOM	3556	CE2	TYR	B	229	49.079	46.940	-4.629	1.00	27.97
ATOM	3557	CD2	TYR	B	229	49.226	48.265	-5.049	1.00	28.17
ATOM	3558	C	TYR	B	229	49.713	51.146	-2.919	1.00	28.17
ATOM	3559	O	TYR	B	229	50.873	50.788	-3.147	1.00	31.19
ATOM	3560	N	ALA	B	230	49.160	51.081	-1.708	1.00	27.08
ATOM	3561	CA	ALA	B	230	49.859	50.512	-0.562	1.00	23.43
ATOM	3562	CB	ALA	B	230	49.444	51.222	0.698	1.00	22.72
ATOM	3563	C	ALA	B	230	49.554	49.024	-0.471	1.00	23.03
ATOM	3564	O	ALA	B	230	48.402	48.633	-0.313	1.00	23.44
ATOM	3565	N	ASN	B	231	50.594	48.202	-0.570	1.00	24.43

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3566	CA	ASN	B	231	50.446	46.747	-0.700	1.00	25.46
ATOM	3567	CB	ASN	B	231	51.751	46.122	-1.224	1.00	29.96
ATOM	3568	CG	ASN	B	231	51.898	46.251	-2.746	1.00	33.44
ATOM	3569	OD1	ASN	B	231	51.525	45.346	-3.511	1.00	33.53
ATOM	3570	ND2	ASN	B	231	52.441	47.381	-3.189	1.00	35.04
ATOM	3571	C	ASN	B	231	49.948	45.981	0.535	1.00	22.34
ATOM	3572	O	ASN	B	231	49.330	44.925	0.398	1.00	21.90
ATOM	3573	N	GLY	B	232	50.205	46.515	1.726	1.00	20.16
ATOM	3574	CA	GLY	B	232	49.874	45.831	2.967	1.00	17.91
ATOM	3575	C	GLY	B	232	48.495	46.116	3.535	1.00	18.47
ATOM	3576	O	GLY	B	232	48.199	45.733	4.673	1.00	17.38
ATOM	3577	N	GLY	B	233	47.655	46.798	2.757	1.00	19.34
ATOM	3578	CA	GLY	B	233	46.279	47.074	3.149	1.00	21.72
ATOM	3579	C	GLY	B	233	46.132	48.004	4.340	1.00	22.37
ATOM	3580	O	GLY	B	233	47.109	48.589	4.803	1.00	23.78
ATOM	3581	N	GLU	B	234	44.904	48.157	4.826	1.00	22.76
ATOM	3582	CA	GLU	B	234	44.651	48.983	6.009	1.00	20.83
ATOM	3583	CB	GLU	B	234	43.159	49.326	6.183	1.00	26.19
ATOM	3584	CG	GLU	B	234	42.202	48.705	5.164	1.00	32.46
ATOM	3585	CD	GLU	B	234	40.778	48.562	5.691	1.00	35.07
ATOM	3586	OE1	GLU	B	234	40.331	47.406	5.904	1.00	36.60
ATOM	3587	OE2	GLU	B	234	40.101	49.600	5.891	1.00	35.06
ATOM	3588	C	GLU	B	234	45.168	48.288	7.249	1.00	16.25
ATOM	3589	O	GLU	B	234	45.318	47.069	7.282	1.00	15.37
ATOM	3590	N	LEU	B	235	45.455	49.083	8.268	1.00	14.75
ATOM	3591	CA	LEU	B	235	45.927	48.567	9.545	1.00	11.98
ATOM	3592	CB	LEU	B	235	46.388	49.712	10.443	1.00	8.14
ATOM	3593	CG	LEU	B	235	47.555	49.400	11.369	1.00	7.64
ATOM	3594	CD1	LEU	B	235	48.578	48.519	10.684	1.00	9.85
ATOM	3595	CD2	LEU	B	235	48.204	50.688	11.821	1.00	8.88
ATOM	3596	C	LEU	B	235	44.798	47.819	10.198	1.00	10.94
ATOM	3597	O	LEU	B	235	45.011	46.847	10.904	1.00	12.43
ATOM	3598	N	PHE	B	236	43.588	48.289	9.933	1.00	10.87
ATOM	3599	CA	PHE	B	236	42.389	47.666	10.425	1.00	11.40
ATOM	3600	CB	PHE	B	236	41.166	48.437	9.937	1.00	12.84
ATOM	3601	CG	PHE	B	236	39.863	47.761	10.249	1.00	16.04
ATOM	3602	CD1	PHE	B	236	39.486	47.520	11.571	1.00	19.00
ATOM	3603	CE1	PHE	B	236	38.290	46.892	11.867	1.00	19.86
ATOM	3604	CZ	PHE	B	236	37.454	46.491	10.832	1.00	21.31
ATOM	3605	CE2	PHE	B	236	37.828	46.716	9.506	1.00	18.80
ATOM	3606	CD2	PHE	B	236	39.023	47.348	9.226	1.00	16.34
ATOM	3607	C	PHE	B	236	42.324	46.213	9.972	1.00	12.66
ATOM	3608	O	PHE	B	236	41.777	45.362	10.674	1.00	14.17
ATOM	3609	N	PHE	B	237	42.879	45.919	8.802	1.00	12.25
ATOM	3610	CA	PHE	B	237	42.913	44.536	8.352	1.00	11.35
ATOM	3611	CB	PHE	B	237	43.495	44.417	6.949	1.00	7.11
ATOM	3612	CG	PHE	B	237	43.428	43.032	6.377	1.00	4.35
ATOM	3613	CD1	PHE	B	237	42.292	42.596	5.709	1.00	3.73
ATOM	3614	CE1	PHE	B	237	42.233	41.329	5.161	1.00	2.00
ATOM	3615	CZ	PHE	B	237	43.311	40.474	5.281	1.00	3.10
ATOM	3616	CE2	PHE	B	237	44.452	40.895	5.940	1.00	4.74
ATOM	3617	CD2	PHE	B	237	44.505	42.170	6.487	1.00	4.37

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3618	C	PHE	B	237	43.743	43.748	9.347	1.00	12.10
ATOM	3619	O	PHE	B	237	43.235	42.847	10.005	1.00	15.18
ATOM	3620	N	HIS	B	238	45.005	44.131	9.486	1.00	12.48
ATOM	3621	CA	HIS	B	238	45.932	43.436	10.362	1.00	12.30
ATOM	3622	CB	HIS	B	238	47.300	44.080	10.286	1.00	13.34
ATOM	3623	CG	HIS	B	238	47.932	43.934	8.950	1.00	16.34
ATOM	3624	ND1	HIS	B	238	48.172	42.702	8.380	1.00	17.77
ATOM	3625	CE1	HIS	B	238	48.718	42.877	7.191	1.00	19.98
ATOM	3626	NE2	HIS	B	238	48.826	44.176	6.966	1.00	20.31
ATOM	3627	CD2	HIS	B	238	48.331	44.859	8.048	1.00	18.37
ATOM	3628	C	HIS	B	238	45.470	43.392	11.795	1.00	12.20
ATOM	3629	O	HIS	B	238	45.637	42.375	12.467	1.00	12.69
ATOM	3630	N	LEU	B	239	44.893	44.490	12.271	1.00	12.45
ATOM	3631	CA	LEU	B	239	44.407	44.502	13.632	1.00	12.24
ATOM	3632	CB	LEU	B	239	44.053	45.898	14.119	1.00	13.26
ATOM	3633	CG	LEU	B	239	44.026	46.021	15.657	1.00	18.81
ATOM	3634	CD1	LEU	B	239	45.123	45.221	16.397	1.00	17.71
ATOM	3635	CD2	LEU	B	239	44.059	47.473	16.107	1.00	20.71
ATOM	3636	C	LEU	B	239	43.242	43.555	13.767	1.00	12.24
ATOM	3637	O	LEU	B	239	43.148	42.859	14.758	1.00	15.41
ATOM	3638	N	SER	B	240	42.393	43.476	12.750	1.00	13.36
ATOM	3639	CA	SER	B	240	41.257	42.568	12.802	1.00	13.98
ATOM	3640	CB	SER	B	240	40.257	42.886	11.705	1.00	14.45
ATOM	3641	OG	SER	B	240	39.239	43.717	12.234	1.00	17.74
ATOM	3642	C	SER	B	240	41.672	41.106	12.759	1.00	17.75
ATOM	3643	O	SER	B	240	41.177	40.299	13.546	1.00	18.66
ATOM	3644	N	ARG	B	241	42.592	40.781	11.853	1.00	23.18
ATOM	3645	CA	ARG	B	241	43.134	39.428	11.704	1.00	25.44
ATOM	3646	CB	ARG	B	241	44.011	39.350	10.445	1.00	28.42
ATOM	3647	CG	ARG	B	241	43.611	38.290	9.401	1.00	34.89
ATOM	3648	CD	ARG	B	241	42.112	37.968	9.317	1.00	38.95
ATOM	3649	NE	ARG	B	241	41.447	38.556	8.148	1.00	41.44
ATOM	3650	CZ	ARG	B	241	41.003	39.814	8.069	1.00	40.91
ATOM	3651	NH1	ARG	B	241	41.153	40.654	9.087	1.00	41.21
ATOM	3652	NH2	ARG	B	241	40.401	40.234	6.963	1.00	39.49
ATOM	3653	C	ARG	B	241	43.927	38.961	12.934	1.00	25.59
ATOM	3654	O	ARG	B	241	43.706	37.862	13.438	1.00	24.73
ATOM	3655	N	GLU	B	242	44.831	39.809	13.422	1.00	27.86
ATOM	3656	CA	GLU	B	242	45.775	39.423	14.472	1.00	29.22
ATOM	3657	CB	GLU	B	242	47.192	39.939	14.132	1.00	32.42
ATOM	3658	CG	GLU	B	242	48.074	38.930	13.379	1.00	38.65
ATOM	3659	CD	GLU	B	242	48.236	39.197	11.867	1.00	43.26
ATOM	3660	OE1	GLU	B	242	48.752	40.283	11.484	1.00	45.59
ATOM	3661	OE2	GLU	B	242	47.884	38.303	11.047	1.00	41.56
ATOM	3662	C	GLU	B	242	45.312	39.811	15.893	1.00	26.73
ATOM	3663	O	GLU	B	242	46.004	39.540	16.879	1.00	25.63
ATOM	3664	N	ARG	B	243	44.133	40.428	15.982	1.00	25.04
ATOM	3665	CA	ARG	B	243	43.449	40.724	17.257	1.00	26.42
ATOM	3666	CB	ARG	B	243	43.157	39.430	18.031	1.00	33.23
ATOM	3667	CG	ARG	B	243	42.671	39.588	19.479	1.00	40.89
ATOM	3668	CD	ARG	B	243	43.052	38.398	20.393	1.00	45.42
ATOM	3669	NE	ARG	B	243	44.511	38.250	20.512	1.00	46.45

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3670	CZ	ARG	B	243	45.163	37.098	20.654	1.00	43.99
ATOM	3671	NH1	ARG	B	243	44.505	35.943	20.705	1.00	42.91
ATOM	3672	NH2	ARG	B	243	46.486	37.110	20.751	1.00	43.20
ATOM	3673	C	ARG	B	243	44.087	41.817	18.145	1.00	23.60
ATOM	3674	O	ARG	B	243	43.430	42.823	18.456	1.00	20.86
ATOM	3675	N	VAL	B	244	45.347	41.640	18.549	1.00	20.80
ATOM	3676	CA	VAL	B	244	46.065	42.714	19.275	1.00	17.32
ATOM	3677	CB	VAL	B	244	45.764	42.675	20.788	1.00	13.75
ATOM	3678	CG1	VAL	B	244	45.957	41.277	21.334	1.00	14.89
ATOM	3679	CG2	VAL	B	244	46.627	43.651	21.519	1.00	14.53
ATOM	3680	C	VAL	B	244	47.594	42.798	19.016	1.00	12.92
ATOM	3681	O	VAL	B	244	48.306	41.813	19.148	1.00	12.72
ATOM	3682	N	PHE	B	245	48.077	43.978	18.640	1.00	8.85
ATOM	3683	CA	PHE	B	245	49.492	44.176	18.359	1.00	7.43
ATOM	3684	CB	PHE	B	245	49.733	45.523	17.693	1.00	6.03
ATOM	3685	CG	PHE	B	245	49.151	45.643	16.329	1.00	7.92
ATOM	3686	CD1	PHE	B	245	48.698	44.516	15.636	1.00	8.46
ATOM	3687	CE1	PHE	B	245	48.147	44.639	14.357	1.00	8.66
ATOM	3688	CZ	PHE	B	245	48.049	45.907	13.764	1.00	10.44
ATOM	3689	CE2	PHE	B	245	48.505	47.042	14.453	1.00	10.03
ATOM	3690	CD2	PHE	B	245	49.051	46.898	15.726	1.00	9.11
ATOM	3691	C	PHE	B	245	50.298	44.154	19.635	1.00	8.25
ATOM	3692	O	PHE	B	245	49.844	44.657	20.658	1.00	10.25
ATOM	3693	N	SER	B	246	51.496	43.574	19.565	1.00	9.03
ATOM	3694	CA	SER	B	246	52.469	43.687	20.636	1.00	10.64
ATOM	3695	CB	SER	B	246	53.743	42.933	20.275	1.00	12.32
ATOM	3696	OG	SER	B	246	54.700	43.797	19.673	1.00	11.12
ATOM	3697	C	SER	B	246	52.789	45.163	20.829	1.00	12.93
ATOM	3698	O	SER	B	246	52.749	45.943	19.875	1.00	11.65
ATOM	3699	N	GLU	B	247	53.116	45.535	22.062	1.00	16.52
ATOM	3700	CA	GLU	B	247	53.413	46.926	22.403	1.00	18.36
ATOM	3701	CB	GLU	B	247	53.854	47.031	23.862	1.00	20.57
ATOM	3702	CG	GLU	B	247	52.992	47.959	24.689	1.00	24.45
ATOM	3703	CD	GLU	B	247	53.340	47.917	26.168	1.00	29.43
ATOM	3704	OE1	GLU	B	247	54.418	48.466	26.545	1.00	29.97
ATOM	3705	OE2	GLU	B	247	52.531	47.337	26.946	1.00	28.87
ATOM	3706	C	GLU	B	247	54.452	47.578	21.485	1.00	19.59
ATOM	3707	O	GLU	B	247	54.296	48.735	21.107	1.00	20.59
ATOM	3708	N	ASP	B	248	55.506	46.845	21.132	1.00	22.07
ATOM	3709	CA	ASP	B	248	56.562	47.392	20.286	1.00	25.41
ATOM	3710	CB	ASP	B	248	57.833	46.533	20.315	1.00	31.95
ATOM	3711	CG	ASP	B	248	58.297	46.200	21.738	1.00	38.78
ATOM	3712	OD1	ASP	B	248	59.536	46.143	21.969	1.00	41.91
ATOM	3713	OD2	ASP	B	248	57.500	45.961	22.682	1.00	41.40
ATOM	3714	C	ASP	B	248	56.043	47.545	18.864	1.00	25.21
ATOM	3715	O	ASP	B	248	56.320	48.553	18.209	1.00	27.38
ATOM	3716	N	ARG	B	249	55.272	46.562	18.392	1.00	21.04
ATOM	3717	CA	ARG	B	249	54.624	46.687	17.094	1.00	16.48
ATOM	3718	CB	ARG	B	249	53.726	45.491	16.787	1.00	20.73
ATOM	3719	CG	ARG	B	249	52.761	45.695	15.606	1.00	24.52
ATOM	3720	CD	ARG	B	249	53.272	45.179	14.265	1.00	26.01
ATOM	3721	NE	ARG	B	249	52.216	44.631	13.412	1.00	26.55

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3722	CZ	ARG	B	249	52.005	43.331	13.232	1.00	29.09
ATOM	3723	NH1	ARG	B	249	52.769	42.434	13.853	1.00	29.90
ATOM	3724	NH2	ARG	B	249	51.029	42.921	12.429	1.00	28.91
ATOM	3725	C	ARG	B	249	53.828	47.977	17.090	1.00	12.59
ATOM	3726	O	ARG	B	249	53.955	48.773	16.172	1.00	15.67
ATOM	3727	N	ALA	B	250	53.035	48.198	18.133	1.00	9.24
ATOM	3728	CA	ALA	B	250	52.304	49.456	18.270	1.00	6.86
ATOM	3729	CB	ALA	B	250	51.380	49.434	19.470	1.00	3.36
ATOM	3730	C	ALA	B	250	53.245	50.649	18.334	1.00	6.78
ATOM	3731	O	ALA	B	250	53.075	51.600	17.577	1.00	9.97
ATOM	3732	N	ARG	B	251	54.249	50.595	19.206	1.00	6.67
ATOM	3733	CA	ARG	B	251	55.145	51.736	19.385	1.00	9.26
ATOM	3734	CB	ARG	B	251	56.273	51.427	20.379	1.00	8.88
ATOM	3735	CG	ARG	B	251	57.471	52.401	20.316	1.00	7.32
ATOM	3736	CD	ARG	B	251	58.390	52.375	21.528	1.00	8.86
ATOM	3737	NE	ARG	B	251	58.726	51.014	21.939	1.00	10.26
ATOM	3738	CZ	ARG	B	251	58.267	50.425	23.040	1.00	9.71
ATOM	3739	NH1	ARG	B	251	57.448	51.073	23.862	1.00	11.36
ATOM	3740	NH2	ARG	B	251	58.624	49.180	23.322	1.00	7.85
ATOM	3741	C	ARG	B	251	55.712	52.188	18.044	1.00	10.47
ATOM	3742	O	ARG	B	251	55.872	53.388	17.806	1.00	10.48
ATOM	3743	N	PHE	B	252	55.992	51.215	17.177	1.00	10.75
ATOM	3744	CA	PHE	B	252	56.560	51.477	15.860	1.00	12.79
ATOM	3745	CB	PHE	B	252	56.930	50.160	15.173	1.00	13.58
ATOM	3746	CG	PHE	B	252	57.263	50.304	13.716	1.00	15.85
ATOM	3747	CD1	PHE	B	252	58.586	50.358	13.300	1.00	16.32
ATOM	3748	CE1	PHE	B	252	58.906	50.487	11.959	1.00	15.62
ATOM	3749	CZ	PHE	B	252	57.894	50.554	11.011	1.00	16.06
ATOM	3750	CE2	PHE	B	252	56.567	50.498	11.412	1.00	17.32
ATOM	3751	CD2	PHE	B	252	56.256	50.368	12.757	1.00	16.07
ATOM	3752	C	PHE	B	252	55.569	52.267	15.018	1.00	13.87
ATOM	3753	O	PHE	B	252	55.872	53.378	14.578	1.00	15.18
ATOM	3754	N	TYR	B	253	54.386	51.686	14.814	1.00	11.93
ATOM	3755	CA	TYR	B	253	53.319	52.332	14.066	1.00	11.73
ATOM	3756	CB	TYR	B	253	52.051	51.451	14.022	1.00	12.04
ATOM	3757	CG	TYR	B	253	52.191	50.173	13.204	1.00	11.95
ATOM	3758	CD1	TYR	B	253	52.843	50.170	11.976	1.00	13.55
ATOM	3759	CE1	TYR	B	253	52.984	49.008	11.224	1.00	15.10
ATOM	3760	CZ	TYR	B	253	52.459	47.821	11.692	1.00	16.33
ATOM	3761	OH	TYR	B	253	52.595	46.660	10.933	1.00	16.01
ATOM	3762	CE2	TYR	B	253	51.796	47.804	12.914	1.00	14.88
ATOM	3763	CD2	TYR	B	253	51.669	48.974	13.660	1.00	11.99
ATOM	3764	C	TYR	B	253	53.031	53.723	14.639	1.00	10.93
ATOM	3765	O	TYR	B	253	52.960	54.700	13.892	1.00	11.26
ATOM	3766	N	GLY	B	254	52.910	53.811	15.962	1.00	9.60
ATOM	3767	CA	GLY	B	254	52.648	55.075	16.626	1.00	8.49
ATOM	3768	C	GLY	B	254	53.728	56.102	16.331	1.00	9.75
ATOM	3769	O	GLY	B	254	53.448	57.268	16.086	1.00	7.16
ATOM	3770	N	ALA	B	255	54.976	55.660	16.342	1.00	11.39
ATOM	3771	CA	ALA	B	255	56.088	56.566	16.140	1.00	13.46
ATOM	3772	CB	ALA	B	255	57.407	55.840	16.346	1.00	16.28
ATOM	3773	C	ALA	B	255	56.015	57.167	14.749	1.00	16.98

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3774	O	ALA	B	255	56.149	58.387	14.595	1.00	19.71
ATOM	3775	N	GLU	B	256	55.789	56.317	13.741	1.00	16.99
ATOM	3776	CA	GLU	B	256	55.700	56.782	12.356	1.00	15.53
ATOM	3777	CB	GLU	B	256	55.694	55.631	11.346	1.00	16.03
ATOM	3778	CG	GLU	B	256	56.682	54.518	11.667	1.00	21.98
ATOM	3779	CD	GLU	B	256	57.471	54.020	10.461	1.00	24.51
ATOM	3780	OE1	GLU	B	256	56.871	53.325	9.606	1.00	24.45
ATOM	3781	OE2	GLU	B	256	58.699	54.298	10.380	1.00	25.10
ATOM	3782	C	GLU	B	256	54.476	57.668	12.193	1.00	15.45
ATOM	3783	O	GLU	B	256	54.541	58.671	11.490	1.00	17.96
ATOM	3784	N	ILE	B	257	53.377	57.314	12.861	1.00	11.95
ATOM	3785	CA	ILE	B	257	52.176	58.148	12.858	1.00	11.20
ATOM	3786	CB	ILE	B	257	51.000	57.455	13.613	1.00	10.84
ATOM	3787	CG1	ILE	B	257	50.575	56.177	12.892	1.00	12.72
ATOM	3788	CD1	ILE	B	257	49.644	55.301	13.704	1.00	13.50
ATOM	3789	CG2	ILE	B	257	49.789	58.376	13.747	1.00	5.24
ATOM	3790	C	ILE	B	257	52.499	59.522	13.453	1.00	11.67
ATOM	3791	O	ILE	B	257	52.212	60.557	12.829	1.00	12.09
ATOM	3792	N	VAL	B	258	53.109	59.516	14.642	1.00	10.87
ATOM	3793	CA	VAL	B	258	53.482	60.737	15.355	1.00	11.46
ATOM	3794	CB	VAL	B	258	54.181	60.448	16.717	1.00	13.08
ATOM	3795	CG1	VAL	B	258	54.782	61.725	17.320	1.00	11.32
ATOM	3796	CG2	VAL	B	258	53.233	59.788	17.712	1.00	11.37
ATOM	3797	C	VAL	B	258	54.428	61.537	14.485	1.00	13.06
ATOM	3798	O	VAL	B	258	54.381	62.768	14.476	1.00	17.71
ATOM	3799	N	SER	B	259	55.281	60.842	13.741	1.00	11.90
ATOM	3800	CA	SER	B	259	56.160	61.528	12.805	1.00	13.92
ATOM	3801	CB	SER	B	259	57.045	60.539	12.056	1.00	14.45
ATOM	3802	OG	SER	B	259	57.933	61.235	11.202	1.00	15.85
ATOM	3803	C	SER	B	259	55.367	62.379	11.812	1.00	13.33
ATOM	3804	O	SER	B	259	55.593	63.586	11.707	1.00	13.14
ATOM	3805	N	ALA	B	260	54.421	61.734	11.125	1.00	12.38
ATOM	3806	CA	ALA	B	260	53.659	62.324	10.025	1.00	9.41
ATOM	3807	CB	ALA	B	260	52.852	61.253	9.321	1.00	8.75
ATOM	3808	C	ALA	B	260	52.751	63.449	10.475	1.00	10.35
ATOM	3809	O	ALA	B	260	52.697	64.497	9.821	1.00	4.53
ATOM	3810	N	LEU	B	261	52.034	63.208	11.580	1.00	13.29
ATOM	3811	CA	LEU	B	261	51.186	64.213	12.230	1.00	16.38
ATOM	3812	CB	LEU	B	261	50.461	63.620	13.437	1.00	20.28
ATOM	3813	CG	LEU	B	261	49.305	62.650	13.190	1.00	24.47
ATOM	3814	CD1	LEU	B	261	49.069	61.799	14.433	1.00	25.71
ATOM	3815	CD2	LEU	B	261	48.028	63.383	12.807	1.00	25.27
ATOM	3816	C	LEU	B	261	51.968	65.452	12.674	1.00	16.26
ATOM	3817	O	LEU	B	261	51.479	66.580	12.556	1.00	15.70
ATOM	3818	N	ASP	B	262	53.177	65.248	13.186	1.00	16.35
ATOM	3819	CA	ASP	B	262	54.037	66.377	13.481	1.00	19.99
ATOM	3820	CB	ASP	B	262	55.360	65.929	14.103	1.00	26.16
ATOM	3821	CG	ASP	B	262	56.248	67.112	14.487	1.00	33.46
ATOM	3822	OD1	ASP	B	262	57.440	67.125	14.103	1.00	36.25
ATOM	3823	OD2	ASP	B	262	55.834	68.092	15.154	1.00	36.48
ATOM	3824	C	ASP	B	262	54.285	67.221	12.220	1.00	18.68
ATOM	3825	O	ASP	B	262	54.294	68.453	12.283	1.00	18.21

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3826	N	TYR	B	263	54.464	66.551	11.081	1.00	17.48
ATOM	3827	CA	TYR	B	263	54.758	67.219	9.809	1.00	15.05
ATOM	3828	CB	TYR	B	263	55.132	66.190	8.738	1.00	15.69
ATOM	3829	CG	TYR	B	263	55.120	66.690	7.301	1.00	14.80
ATOM	3830	CD1	TYR	B	263	56.275	67.195	6.704	1.00	15.24
ATOM	3831	CE1	TYR	B	263	56.272	67.636	5.373	1.00	13.92
ATOM	3832	CZ	TYR	B	263	55.102	67.565	4.636	1.00	12.27
ATOM	3833	OH	TYR	B	263	55.075	67.993	3.334	1.00	9.40
ATOM	3834	CE2	TYR	B	263	53.949	67.061	5.207	1.00	13.72
ATOM	3835	CD2	TYR	B	263	53.964	66.620	6.527	1.00	14.46
ATOM	3836	C	TYR	B	263	53.603	68.086	9.336	1.00	11.49
ATOM	3837	O	TYR	B	263	53.830	69.195	8.866	1.00	10.76
ATOM	3838	N	LEU	B	264	52.381	67.565	9.461	1.00	7.44
ATOM	3839	CA	LEU	B	264	51.177	68.272	9.047	1.00	6.41
ATOM	3840	CB	LEU	B	264	49.980	67.324	8.965	1.00	5.17
ATOM	3841	CG	LEU	B	264	50.126	66.107	8.047	1.00	4.42
ATOM	3842	CD1	LEU	B	264	49.436	64.900	8.658	1.00	4.41
ATOM	3843	CD2	LEU	B	264	49.581	66.396	6.659	1.00	2.79
ATOM	3844	C	LEU	B	264	50.866	69.424	9.986	1.00	9.34
ATOM	3845	O	LEU	B	264	50.503	70.514	9.530	1.00	8.84
ATOM	3846	N	HIS	B	265	51.021	69.192	11.291	1.00	12.24
ATOM	3847	CA	HIS	B	265	50.812	70.253	12.279	1.00	15.69
ATOM	3848	CB	HIS	B	265	50.942	69.724	13.693	1.00	15.73
ATOM	3849	CG	HIS	B	265	49.743	68.976	14.166	1.00	18.99
ATOM	3850	ND1	HIS	B	265	49.481	68.762	15.502	1.00	19.56
ATOM	3851	CE1	HIS	B	265	48.364	68.065	15.620	1.00	21.56
ATOM	3852	NE2	HIS	B	265	47.891	67.821	14.410	1.00	21.71
ATOM	3853	CD2	HIS	B	265	48.736	68.380	13.482	1.00	20.73
ATOM	3854	C	HIS	B	265	51.761	71.424	12.095	1.00	17.80
ATOM	3855	O	HIS	B	265	51.413	72.551	12.429	1.00	18.90
ATOM	3856	N	SER	B	266	52.953	71.146	11.571	1.00	20.25
ATOM	3857	CA	SER	B	266	53.938	72.182	11.261	1.00	22.04
ATOM	3858	CB	SER	B	266	55.338	71.591	11.155	1.00	22.97
ATOM	3859	OG	SER	B	266	55.662	70.896	12.340	1.00	26.79
ATOM	3860	C	SER	B	266	53.607	72.911	9.975	1.00	22.21
ATOM	3861	O	SER	B	266	53.963	74.076	9.830	1.00	22.23
ATOM	3862	N	ARG	B	267	52.948	72.218	9.043	1.00	22.84
ATOM	3863	CA	ARG	B	267	52.465	72.837	7.803	1.00	24.70
ATOM	3864	CB	ARG	B	267	52.504	71.861	6.612	1.00	24.20
ATOM	3865	CG	ARG	B	267	53.859	71.205	6.320	1.00	24.57
ATOM	3866	CD	ARG	B	267	54.696	71.860	5.223	1.00	26.75
ATOM	3867	NE	ARG	B	267	54.068	71.823	3.902	1.00	28.96
ATOM	3868	CZ	ARG	B	267	54.688	72.117	2.755	1.00	31.17
ATOM	3869	NH1	ARG	B	267	55.974	72.466	2.738	1.00	31.08
ATOM	3870	NH2	ARG	B	267	54.018	72.061	1.612	1.00	31.93
ATOM	3871	C	ARG	B	267	51.050	73.401	8.002	1.00	26.83
ATOM	3872	O	ARG	B	267	50.373	73.790	7.037	1.00	26.30
ATOM	3873	N	ASP	B	268	50.616	73.431	9.264	1.00	28.62
ATOM	3874	CA	ASP	B	268	49.358	74.064	9.677	1.00	29.79
ATOM	3875	CB	ASP	B	268	49.197	75.445	9.025	1.00	31.20
ATOM	3876	CG	ASP	B	268	50.113	76.491	9.635	1.00	33.22
ATOM	3877	OD1	ASP	B	268	50.358	76.424	10.861	1.00	33.13

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3878	OD2	ASP	B	268	50.626	77.422	8.966	1.00	35.06
ATOM	3879	C	ASP	B	268	48.113	73.215	9.428	1.00	28.67
ATOM	3880	O	ASP	B	268	46.992	73.643	9.715	1.00	29.73
ATOM	3881	N	VAL	B	269	48.317	72.013	8.901	1.00	25.09
ATOM	3882	CA	VAL	B	269	47.216	71.121	8.585	1.00	21.13
ATOM	3883	CB	VAL	B	269	47.597	70.122	7.480	1.00	20.59
ATOM	3884	CG1	VAL	B	269	46.391	69.296	7.064	1.00	20.48
ATOM	3885	CG2	VAL	B	269	48.187	70.846	6.280	1.00	21.56
ATOM	3886	C	VAL	B	269	46.835	70.344	9.824	1.00	20.15
ATOM	3887	O	VAL	B	269	47.710	69.838	10.530	1.00	23.42
ATOM	3888	N	VAL	B	270	45.536	70.253	10.093	1.00	16.48
ATOM	3889	CA	VAL	B	270	45.034	69.315	11.095	1.00	14.10
ATOM	3890	CB	VAL	B	270	44.104	69.999	12.100	1.00	12.84
ATOM	3891	CG1	VAL	B	270	43.569	68.993	13.113	1.00	11.27
ATOM	3892	CG2	VAL	B	270	44.849	71.116	12.802	1.00	11.59
ATOM	3893	C	VAL	B	270	44.351	68.148	10.372	1.00	13.41
ATOM	3894	O	VAL	B	270	43.500	68.371	9.496	1.00	13.88
ATOM	3895	N	TYR	B	271	44.743	66.916	10.717	1.00	8.60
ATOM	3896	CA	TYR	B	271	44.361	65.769	9.911	1.00	6.61
ATOM	3897	CB	TYR	B	271	45.191	64.555	10.211	1.00	6.33
ATOM	3898	CG	TYR	B	271	44.714	63.318	9.478	1.00	9.70
ATOM	3899	CD1	TYR	B	271	44.680	63.271	8.082	1.00	8.67
ATOM	3900	CE1	TYR	B	271	44.250	62.128	7.417	1.00	9.99
ATOM	3901	CZ	TYR	B	271	43.857	61.013	8.154	1.00	10.62
ATOM	3902	OH	TYR	B	271	43.435	59.873	7.516	1.00	11.89
ATOM	3903	CE2	TYR	B	271	43.887	61.030	9.534	1.00	9.27
ATOM	3904	CD2	TYR	B	271	44.306	62.178	10.187	1.00	11.18
ATOM	3905	C	TYR	B	271	42.920	65.442	10.110	1.00	8.64
ATOM	3906	O	TYR	B	271	42.176	65.317	9.136	1.00	14.24
ATOM	3907	N	ARG	B	272	42.540	65.276	11.369	1.00	8.63
ATOM	3908	CA	ARG	B	272	41.139	65.364	11.771	1.00	10.79
ATOM	3909	CB	ARG	B	272	40.489	66.581	11.112	1.00	8.64
ATOM	3910	CG	ARG	B	272	39.812	67.526	12.048	1.00	8.05
ATOM	3911	CD	ARG	B	272	38.499	68.043	11.508	1.00	8.63
ATOM	3912	NE	ARG	B	272	38.660	68.690	10.208	1.00	7.20
ATOM	3913	CZ	ARG	B	272	38.070	69.825	9.846	1.00	5.40
ATOM	3914	NH1	ARG	B	272	37.255	70.463	10.680	1.00	3.22
ATOM	3915	NH2	ARG	B	272	38.295	70.322	8.635	1.00	4.22
ATOM	3916	C	ARG	B	272	40.297	64.133	11.491	1.00	13.52
ATOM	3917	O	ARG	B	272	39.080	64.217	11.497	1.00	17.96
ATOM	3918	N	ASP	B	273	40.928	62.997	11.239	1.00	18.21
ATOM	3919	CA	ASP	B	273	40.179	61.755	11.076	1.00	26.05
ATOM	3920	CB	ASP	B	273	39.440	61.725	9.729	1.00	27.64
ATOM	3921	CG	ASP	B	273	38.417	60.588	9.645	1.00	32.74
ATOM	3922	OD1	ASP	B	273	37.912	60.147	10.709	1.00	34.89
ATOM	3923	OD2	ASP	B	273	38.074	60.059	8.559	1.00	34.29
ATOM	3924	C	ASP	B	273	41.030	60.484	11.280	1.00	30.86
ATOM	3925	O	ASP	B	273	40.929	59.512	10.511	1.00	31.97
ATOM	3926	N	LEU	B	274	41.856	60.476	12.325	1.00	29.70
ATOM	3927	CA	LEU	B	274	42.631	59.281	12.616	1.00	25.23
ATOM	3928	CB	LEU	B	274	43.540	59.501	13.832	1.00	24.15
ATOM	3929	CG	LEU	B	274	44.972	59.912	13.465	1.00	23.29

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3930	CD1	LEU	B	274	45.547	60.841	14.484	1.00	24.64
ATOM	3931	CD2	LEU	B	274	45.870	58.716	13.324	1.00	23.16
ATOM	3932	C	LEU	B	274	41.687	58.074	12.785	1.00	23.84
ATOM	3933	O	LEU	B	274	40.551	58.215	13.272	1.00	23.21
ATOM	3934	N	LYS	B	275	42.149	56.917	12.312	1.00	19.54
ATOM	3935	CA	LYS	B	275	41.452	55.635	12.440	1.00	14.94
ATOM	3936	CB	LYS	B	275	40.013	55.687	11.915	1.00	15.47
ATOM	3937	CG	LYS	B	275	39.860	55.855	10.423	1.00	13.62
ATOM	3938	CD	LYS	B	275	38.728	56.806	10.129	1.00	13.95
ATOM	3939	CE	LYS	B	275	37.932	56.339	8.928	1.00	13.96
ATOM	3940	NZ	LYS	B	275	36.602	55.797	9.294	1.00	13.42
ATOM	3941	C	LYS	B	275	42.222	54.580	11.691	1.00	13.50
ATOM	3942	O	LYS	B	275	42.942	54.889	10.751	1.00	14.43
ATOM	3943	N	LEU	B	276	42.061	53.331	12.102	1.00	13.70
ATOM	3944	CA	LEU	B	276	42.824	52.244	11.517	1.00	13.52
ATOM	3945	CB	LEU	B	276	42.473	50.926	12.183	1.00	16.85
ATOM	3946	CG	LEU	B	276	42.570	50.910	13.698	1.00	18.11
ATOM	3947	CD1	LEU	B	276	41.902	49.639	14.204	1.00	20.40
ATOM	3948	CD2	LEU	B	276	44.031	51.012	14.134	1.00	15.92
ATOM	3949	C	LEU	B	276	42.524	52.161	10.050	1.00	11.42
ATOM	3950	O	LEU	B	276	43.427	52.129	9.237	1.00	11.05
ATOM	3951	N	GLU	B	277	41.237	52.141	9.732	1.00	12.97
ATOM	3952	CA	GLU	B	277	40.746	52.189	8.365	1.00	13.31
ATOM	3953	CB	GLU	B	277	39.334	52.774	8.347	1.00	15.76
ATOM	3954	CG	GLU	B	277	38.255	51.811	8.785	1.00	20.20
ATOM	3955	CD	GLU	B	277	38.079	51.761	10.288	1.00	26.93
ATOM	3956	OE1	GLU	B	277	38.930	52.316	11.033	1.00	31.26
ATOM	3957	OE2	GLU	B	277	37.077	51.155	10.731	1.00	30.26
ATOM	3958	C	GLU	B	277	41.632	53.047	7.491	1.00	11.94
ATOM	3959	O	GLU	B	277	41.923	52.668	6.355	1.00	10.81
ATOM	3960	N	ASN	B	278	42.059	54.190	8.037	1.00	9.53
ATOM	3961	CA	ASN	B	278	42.783	55.206	7.280	1.00	11.45
ATOM	3962	CB	ASN	B	278	42.370	56.614	7.720	1.00	12.57
ATOM	3963	CG	ASN	B	278	41.105	57.114	7.012	1.00	15.14
ATOM	3964	OD1	ASN	B	278	40.489	56.394	6.211	1.00	18.84
ATOM	3965	ND2	ASN	B	278	40.713	58.356	7.303	1.00	11.94
ATOM	3966	C	ASN	B	278	44.308	55.072	7.261	1.00	14.22
ATOM	3967	O	ASN	B	278	44.950	55.585	6.356	1.00	21.17
ATOM	3968	N	LEU	B	279	44.897	54.393	8.239	1.00	14.52
ATOM	3969	CA	LEU	B	279	46.334	54.117	8.189	1.00	14.22
ATOM	3970	CB	LEU	B	279	46.900	53.880	9.591	1.00	14.21
ATOM	3971	CG	LEU	B	279	46.348	54.817	10.671	1.00	16.90
ATOM	3972	CD1	LEU	B	279	46.535	54.220	12.044	1.00	17.27
ATOM	3973	CD2	LEU	B	279	46.961	56.214	10.610	1.00	18.37
ATOM	3974	C	LEU	B	279	46.626	52.926	7.282	1.00	15.24
ATOM	3975	O	LEU	B	279	46.070	51.847	7.470	1.00	18.52
ATOM	3976	N	MET	B	280	47.495	53.126	6.299	1.00	14.57
ATOM	3977	CA	MET	B	280	47.873	52.060	5.370	1.00	16.22
ATOM	3978	CB	MET	B	280	47.746	52.563	3.937	1.00	19.44
ATOM	3979	CG	MET	B	280	46.373	53.065	3.572	1.00	21.86
ATOM	3980	SD	MET	B	280	45.226	51.715	3.443	1.00	25.77
ATOM	3981	CE	MET	B	280	46.062	50.624	2.357	1.00	25.16

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	3982	C	MET	B	280	49.292	51.502	5.589	1.00	15.01
ATOM	3983	O	MET	B	280	50.141	52.143	6.208	1.00	16.82
ATOM	3984	N	LEU	B	281	49.540	50.305	5.070	1.00	11.33
ATOM	3985	CA	LEU	B	281	50.876	49.735	5.090	1.00	10.44
ATOM	3986	CB	LEU	B	281	50.875	48.366	5.775	1.00	11.60
ATOM	3987	CG	LEU	B	281	50.898	48.260	7.304	1.00	12.47
ATOM	3988	CD1	LEU	B	281	51.413	46.885	7.740	1.00	11.32
ATOM	3989	CD2	LEU	B	281	51.720	49.371	7.941	1.00	13.97
ATOM	3990	C	LEU	B	281	51.404	49.610	3.669	1.00	11.00
ATOM	3991	O	LEU	B	281	50.699	49.133	2.776	1.00	7.94
ATOM	3992	N	ASP	B	282	52.645	50.048	3.462	1.00	13.47
ATOM	3993	CA	ASP	B	282	53.280	49.940	2.154	1.00	15.45
ATOM	3994	CB	ASP	B	282	54.068	51.220	1.784	1.00	18.66
ATOM	3995	CG	ASP	B	282	55.308	51.445	2.651	1.00	21.95
ATOM	3996	OD1	ASP	B	282	55.692	50.533	3.419	1.00	23.53
ATOM	3997	OD2	ASP	B	282	55.973	52.513	2.614	1.00	21.81
ATOM	3998	C	ASP	B	282	54.106	48.653	2.032	1.00	15.47
ATOM	3999	O	ASP	B	282	54.371	47.980	3.031	1.00	11.94
ATOM	4000	N	LYS	B	283	54.495	48.323	0.800	1.00	18.41
ATOM	4001	CA	LYS	B	283	55.125	47.038	0.470	1.00	20.20
ATOM	4002	CB	LYS	B	283	55.541	47.002	-1.012	1.00	22.65
ATOM	4003	CG	LYS	B	283	56.903	47.637	-1.330	1.00	25.28
ATOM	4004	CD	LYS	B	283	56.853	49.169	-1.290	1.00	27.19
ATOM	4005	CE	LYS	B	283	57.721	49.778	-2.380	1.00	28.25
ATOM	4006	NZ	LYS	B	283	58.863	50.544	-1.807	1.00	28.78
ATOM	4007	C	LYS	B	283	56.304	46.651	1.365	1.00	18.36
ATOM	4008	O	LYS	B	283	56.758	45.512	1.324	1.00	17.22
ATOM	4009	N	ASP	B	284	56.787	47.596	2.164	1.00	17.64
ATOM	4010	CA	ASP	B	284	57.940	47.361	3.023	1.00	20.57
ATOM	4011	CB	ASP	B	284	58.921	48.542	2.949	1.00	22.45
ATOM	4012	CG	ASP	B	284	60.009	48.355	1.881	1.00	24.12
ATOM	4013	OD1	ASP	B	284	60.380	47.199	1.562	1.00	24.05
ATOM	4014	OD2	ASP	B	284	60.559	49.323	1.308	1.00	24.11
ATOM	4015	C	ASP	B	284	57.550	47.080	4.477	1.00	21.72
ATOM	4016	O	ASP	B	284	58.292	46.418	5.206	1.00	25.04
ATOM	4017	N	GLY	B	285	56.389	47.572	4.896	1.00	19.99
ATOM	4018	CA	GLY	B	285	55.974	47.458	6.281	1.00	16.00
ATOM	4019	C	GLY	B	285	55.768	48.820	6.910	1.00	14.30
ATOM	4020	O	GLY	B	285	55.392	48.926	8.080	1.00	13.46
ATOM	4021	N	HIS	B	286	56.000	49.863	6.120	1.00	14.12
ATOM	4022	CA	HIS	B	286	55.938	51.236	6.613	1.00	14.76
ATOM	4023	CB	HIS	B	286	57.035	52.107	5.988	1.00	14.04
ATOM	4024	CG	HIS	B	286	58.404	51.778	6.493	1.00	13.46
ATOM	4025	ND1	HIS	B	286	58.970	52.412	7.576	1.00	13.99
ATOM	4026	CE1	HIS	B	286	60.165	51.903	7.809	1.00	12.21
ATOM	4027	NE2	HIS	B	286	60.388	50.949	6.924	1.00	12.71
ATOM	4028	CD2	HIS	B	286	59.300	50.848	6.093	1.00	12.57
ATOM	4029	C	HIS	B	286	54.567	51.875	6.460	1.00	14.95
ATOM	4030	O	HIS	B	286	53.808	51.599	5.529	1.00	14.87
ATOM	4031	N	ILE	B	287	54.266	52.727	7.420	1.00	15.50
ATOM	4032	CA	ILE	B	287	52.984	53.368	7.512	1.00	16.67
ATOM	4033	CB	ILE	B	287	52.923	54.114	8.860	1.00	17.31

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4034	CG1	ILE	B	287	52.628	53.124	9.997	1.00	16.61
ATOM	4035	CD1	ILE	B	287	51.155	52.943	10.339	1.00	19.28
ATOM	4036	CG2	ILE	B	287	51.969	55.328	8.809	1.00	19.59
ATOM	4037	C	ILE	B	287	52.812	54.311	6.338	1.00	18.26
ATOM	4038	O	ILE	B	287	53.778	54.893	5.848	1.00	21.65
ATOM	4039	N	LYS	B	288	51.582	54.408	5.859	1.00	18.75
ATOM	4040	CA	LYS	B	288	51.164	55.522	5.026	1.00	20.21
ATOM	4041	CB	LYS	B	288	51.024	55.100	3.558	1.00	21.22
ATOM	4042	CG	LYS	B	288	52.327	54.753	2.847	1.00	22.42
ATOM	4043	CD	LYS	B	288	53.173	55.987	2.622	1.00	22.79
ATOM	4044	CE	LYS	B	288	54.265	55.706	1.619	1.00	24.52
ATOM	4045	NZ	LYS	B	288	54.815	56.972	1.038	1.00	25.89
ATOM	4046	C	LYS	B	288	49.820	55.981	5.569	1.00	19.61
ATOM	4047	O	LYS	B	288	48.972	55.153	5.903	1.00	20.57
ATOM	4048	N	ILE	B	289	49.618	57.286	5.692	1.00	17.64
ATOM	4049	CA	ILE	B	289	48.271	57.772	5.946	1.00	14.96
ATOM	4050	CB	ILE	B	289	48.247	59.031	6.818	1.00	12.67
ATOM	4051	CG1	ILE	B	289	49.121	58.861	8.052	1.00	13.19
ATOM	4052	CD1	ILE	B	289	49.475	60.180	8.710	1.00	15.81
ATOM	4053	CG2	ILE	B	289	46.816	59.337	7.243	1.00	11.80
ATOM	4054	C	ILE	B	289	47.620	58.060	4.604	1.00	15.91
ATOM	4055	O	ILE	B	289	48.262	58.595	3.699	1.00	15.73
ATOM	4056	N	THR	B	290	46.355	57.676	4.483	1.00	14.99
ATOM	4057	CA	THR	B	290	45.519	58.087	3.374	1.00	17.72
ATOM	4058	CB	THR	B	290	45.120	56.873	2.530	1.00	21.24
ATOM	4059	OG1	THR	B	290	44.450	57.320	1.334	1.00	25.71
ATOM	4060	CG2	THR	B	290	44.070	56.019	3.261	1.00	21.21
ATOM	4061	C	THR	B	290	44.282	58.821	3.896	1.00	17.37
ATOM	4062	O	THR	B	290	44.150	59.036	5.095	1.00	20.44
ATOM	4063	N	ASP	B	291	43.397	59.213	2.981	1.00	16.74
ATOM	4064	CA	ASP	B	291	42.109	59.819	3.300	1.00	12.53
ATOM	4065	CB	ASP	B	291	41.218	58.819	4.021	1.00	8.46
ATOM	4066	CG	ASP	B	291	39.751	59.126	3.863	1.00	7.11
ATOM	4067	OD1	ASP	B	291	39.346	59.579	2.777	1.00	6.11
ATOM	4068	OD2	ASP	B	291	38.914	58.940	4.773	1.00	5.63
ATOM	4069	C	ASP	B	291	42.220	61.138	4.065	1.00	15.34
ATOM	4070	O	ASP	B	291	41.889	61.228	5.245	1.00	14.83
ATOM	4071	N	PHE	B	292	42.693	62.160	3.357	1.00	21.28
ATOM	4072	CA	PHE	B	292	42.773	63.527	3.866	1.00	23.85
ATOM	4073	CB	PHE	B	292	43.940	64.265	3.214	1.00	24.42
ATOM	4074	CG	PHE	B	292	45.255	63.587	3.387	1.00	28.01
ATOM	4075	CD1	PHE	B	292	45.650	62.576	2.520	1.00	30.07
ATOM	4076	CE1	PHE	B	292	46.881	61.947	2.679	1.00	32.33
ATOM	4077	CZ	PHE	B	292	47.735	62.334	3.717	1.00	31.47
ATOM	4078	CE2	PHE	B	292	47.351	63.346	4.581	1.00	30.21
ATOM	4079	CD2	PHE	B	292	46.112	63.965	4.412	1.00	29.79
ATOM	4080	C	PHE	B	292	41.490	64.299	3.575	1.00	24.92
ATOM	4081	O	PHE	B	292	41.480	65.529	3.622	1.00	25.78
ATOM	4082	N	GLY	B	293	40.409	63.576	3.287	1.00	25.90
ATOM	4083	CA	GLY	B	293	39.165	64.182	2.841	1.00	26.17
ATOM	4084	C	GLY	B	293	38.466	65.055	3.861	1.00	25.59
ATOM	4085	O	GLY	B	293	37.377	65.551	3.605	1.00	25.62

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4086	N	LEU	B	294	39.097	65.234	5.017	1.00	26.69
ATOM	4087	CA	LEU	B	294	38.504	65.951	6.136	1.00	27.18
ATOM	4088	CB	LEU	B	294	37.788	64.968	7.073	1.00	27.17
ATOM	4089	CG	LEU	B	294	36.843	63.981	6.376	1.00	27.36
ATOM	4090	CD1	LEU	B	294	37.255	62.528	6.618	1.00	25.96
ATOM	4091	CD2	LEU	B	294	35.385	64.248	6.742	1.00	26.88
ATOM	4092	C	LEU	B	294	39.589	66.716	6.881	1.00	27.27
ATOM	4093	O	LEU	B	294	39.498	66.940	8.083	1.00	28.32
ATOM	4094	N	CYS	B	295	40.623	67.110	6.152	1.00	28.61
ATOM	4095	CA	CYS	B	295	41.716	67.875	6.729	1.00	30.95
ATOM	4096	CB	CYS	B	295	42.960	67.762	5.856	1.00	33.50
ATOM	4097	SG	CYS	B	295	43.930	66.270	6.153	1.00	39.30
ATOM	4098	C	CYS	B	295	41.312	69.326	6.817	1.00	29.29
ATOM	4099	O	CYS	B	295	40.406	69.757	6.112	1.00	31.89
ATOM	4100	N	LYS	B	296	41.972	70.075	7.691	1.00	26.61
ATOM	4101	CA	LYS	B	296	41.807	71.518	7.703	1.00	24.06
ATOM	4102	CB	LYS	B	296	41.115	72.003	8.976	1.00	20.64
ATOM	4103	CG	LYS	B	296	40.703	73.472	8.923	1.00	18.81
ATOM	4104	CD	LYS	B	296	39.201	73.650	8.771	1.00	17.08
ATOM	4105	CE	LYS	B	296	38.845	75.045	8.266	1.00	14.88
ATOM	4106	NZ	LYS	B	296	37.760	75.011	7.242	1.00	11.00
ATOM	4107	C	LYS	B	296	43.160	72.175	7.537	1.00	25.69
ATOM	4108	O	LYS	B	296	44.066	71.959	8.342	1.00	27.64
ATOM	4109	N	GLU	B	297	43.280	72.959	6.468	1.00	27.06
ATOM	4110	CA	GLU	B	297	44.476	73.732	6.158	1.00	27.73
ATOM	4111	CB	GLU	B	297	44.527	74.032	4.651	1.00	30.44
ATOM	4112	CG	GLU	B	297	45.335	73.045	3.810	1.00	33.05
ATOM	4113	CD	GLU	B	297	45.751	73.610	2.453	1.00	34.35
ATOM	4114	OE1	GLU	B	297	46.973	73.746	2.194	1.00	33.32
ATOM	4115	OE2	GLU	B	297	44.853	73.911	1.638	1.00	35.78
ATOM	4116	C	GLU	B	297	44.448	75.046	6.928	1.00	26.90
ATOM	4117	O	GLU	B	297	43.383	75.516	7.327	1.00	27.34
ATOM	4118	N	GLY	B	298	45.621	75.633	7.138	1.00	26.49
ATOM	4119	CA	GLY	B	298	45.710	76.994	7.640	1.00	28.04
ATOM	4120	C	GLY	B	298	45.461	77.194	9.125	1.00	28.16
ATOM	4121	O	GLY	B	298	45.290	78.332	9.577	1.00	26.15
ATOM	4122	N	ILE	B	299	45.441	76.097	9.881	1.00	28.82
ATOM	4123	CA	ILE	B	299	45.351	76.169	11.337	1.00	30.02
ATOM	4124	CB	ILE	B	299	44.813	74.829	11.918	1.00	28.71
ATOM	4125	CG1	ILE	B	299	43.393	74.548	11.413	1.00	28.14
ATOM	4126	CD1	ILE	B	299	42.433	75.726	11.512	1.00	27.71
ATOM	4127	CG2	ILE	B	299	44.870	74.801	13.456	1.00	28.80
ATOM	4128	C	ILE	B	299	46.726	76.535	11.907	1.00	32.40
ATOM	4129	O	ILE	B	299	47.582	75.667	12.097	1.00	34.75
ATOM	4130	N	LYS	B	300	46.940	77.827	12.155	1.00	33.00
ATOM	4131	CA	LYS	B	300	48.208	78.306	12.699	1.00	34.66
ATOM	4132	CB	LYS	B	300	48.442	79.771	12.301	1.00	33.37
ATOM	4133	CG	LYS	B	300	49.212	79.954	10.994	1.00	31.98
ATOM	4134	CD	LYS	B	300	49.691	81.392	10.827	1.00	30.75
ATOM	4135	CE	LYS	B	300	49.703	81.822	9.361	1.00	29.78
ATOM	4136	NZ	LYS	B	300	50.639	82.964	9.100	1.00	27.39
ATOM	4137	C	LYS	B	300	48.249	78.130	14.224	1.00	37.69

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4138	O	LYS	B	300	47.430	77.397	14.785	1.00	37.82
ATOM	4139	N	ASP	B	301	49.225	78.778	14.868	1.00	41.28
ATOM	4140	CA	ASP	B	301	49.314	78.931	16.336	1.00	42.05
ATOM	4141	CB	ASP	B	301	48.979	80.386	16.733	1.00	42.76
ATOM	4142	CG	ASP	B	301	50.214	81.265	16.883	1.00	42.64
ATOM	4143	OD1	ASP	B	301	50.670	81.463	18.031	1.00	42.06
ATOM	4144	OD2	ASP	B	301	50.782	81.818	15.916	1.00	42.92
ATOM	4145	C	ASP	B	301	48.434	77.961	17.141	1.00	41.09
ATOM	4146	O	ASP	B	301	48.868	76.873	17.519	1.00	39.01
ATOM	4147	N	GLY	B	302	47.197	78.383	17.396	1.00	40.84
ATOM	4148	CA	GLY	B	302	46.216	77.577	18.093	1.00	40.09
ATOM	4149	C	GLY	B	302	44.827	77.730	17.497	1.00	39.23
ATOM	4150	O	GLY	B	302	43.904	77.038	17.932	1.00	41.07
ATOM	4151	N	ALA	B	303	44.695	78.617	16.501	1.00	35.74
ATOM	4152	CA	ALA	B	303	43.420	78.938	15.832	1.00	33.12
ATOM	4153	CB	ALA	B	303	43.676	79.655	14.514	1.00	33.92
ATOM	4154	C	ALA	B	303	42.496	77.736	15.614	1.00	30.93
ATOM	4155	O	ALA	B	303	42.942	76.656	15.227	1.00	31.89
ATOM	4156	N	THR	B	304	41.203	77.948	15.847	1.00	28.15
ATOM	4157	CA	THR	B	304	40.247	76.853	16.035	1.00	25.09
ATOM	4158	CB	THR	B	304	39.228	77.240	17.126	1.00	24.05
ATOM	4159	OG1	THR	B	304	39.291	78.651	17.370	1.00	20.65
ATOM	4160	CG2	THR	B	304	39.625	76.628	18.466	1.00	25.55
ATOM	4161	C	THR	B	304	39.499	76.405	14.782	1.00	24.59
ATOM	4162	O	THR	B	304	39.200	77.215	13.901	1.00	28.47
ATOM	4163	N	MET	B	305	39.191	75.112	14.717	1.00	21.30
ATOM	4164	CA	MET	B	305	38.301	74.582	13.685	1.00	21.40
ATOM	4165	CB	MET	B	305	38.683	73.154	13.327	1.00	25.58
ATOM	4166	CG	MET	B	305	39.904	73.025	12.450	1.00	29.28
ATOM	4167	SD	MET	B	305	40.799	71.510	12.828	1.00	33.34
ATOM	4168	CE	MET	B	305	41.805	72.106	14.169	1.00	35.80
ATOM	4169	C	MET	B	305	36.854	74.609	14.169	1.00	17.85
ATOM	4170	O	MET	B	305	36.603	74.754	15.361	1.00	16.79
ATOM	4171	N	LYS	B	306	35.904	74.461	13.250	1.00	15.67
ATOM	4172	CA	LYS	B	306	34.493	74.577	13.610	1.00	13.80
ATOM	4173	CB	LYS	B	306	33.920	75.908	13.112	1.00	15.58
ATOM	4174	CG	LYS	B	306	34.359	77.130	13.927	1.00	14.93
ATOM	4175	CD	LYS	B	306	33.222	78.134	14.093	1.00	13.99
ATOM	4176	CE	LYS	B	306	33.349	78.925	15.397	1.00	13.21
ATOM	4177	NZ	LYS	B	306	32.097	78.914	16.214	1.00	11.81
ATOM	4178	C	LYS	B	306	33.613	73.403	13.165	1.00	13.20
ATOM	4179	O	LYS	B	306	32.654	73.072	13.852	1.00	12.73
ATOM	4180	N	TPO	B	307	33.949	72.771	12.038	1.00	13.75
ATOM	4181	CA	TPO	B	307	33.158	71.664	11.474	1.00	13.74
ATOM	4182	CB	TPO	B	307	33.732	71.229	10.114	1.00	13.15
ATOM	4183	CG2	TPO	B	307	32.815	70.259	9.372	1.00	14.66
ATOM	4184	OG1	TPO	B	307	33.938	72.346	9.253	1.00	10.91
ATOM	4185	P	TPO	B	307	35.420	72.802	8.842	1.00	9.53
ATOM	4186	O1P	TPO	B	307	36.207	71.536	8.300	1.00	6.89
ATOM	4187	O3P	TPO	B	307	35.357	73.859	7.649	1.00	11.73
ATOM	4188	O2P	TPO	B	307	36.108	73.496	10.100	1.00	7.85
ATOM	4189	C	TPO	B	307	33.049	70.458	12.388	1.00	14.07

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4190	O	TPO	B	307	34.050	69.936	12.863	1.00	12.48
ATOM	4191	N	PHE	B	308	31.811	70.019	12.627	1.00	14.74
ATOM	4192	CA	PHE	B	308	31.527	68.786	13.368	1.00	14.01
ATOM	4193	CB	PHE	B	308	30.113	68.827	13.954	1.00	14.29
ATOM	4194	CG	PHE	B	308	29.626	67.514	14.528	1.00	14.25
ATOM	4195	CD1	PHE	B	308	28.531	66.861	13.969	1.00	13.68
ATOM	4196	CE1	PHE	B	308	28.052	65.660	14.501	1.00	11.04
ATOM	4197	CZ	PHE	B	308	28.653	65.112	15.606	1.00	9.76
ATOM	4198	CE2	PHE	B	308	29.732	65.754	16.188	1.00	12.82
ATOM	4199	CD2	PHE	B	308	30.214	66.957	15.652	1.00	14.98
ATOM	4200	C	PHE	B	308	31.680	67.654	12.381	1.00	13.56
ATOM	4201	O	PHE	B	308	30.901	67.529	11.437	1.00	14.83
ATOM	4202	N	CYS	B	309	32.721	66.860	12.581	1.00	13.32
ATOM	4203	CA	CYS	B	309	33.156	65.895	11.586	1.00	14.09
ATOM	4204	CB	CYS	B	309	33.565	66.593	10.283	1.00	11.67
ATOM	4205	SG	CYS	B	309	35.302	67.070	10.197	1.00	10.79
ATOM	4206	C	CYS	B	309	34.307	65.054	12.110	1.00	16.69
ATOM	4207	O	CYS	B	309	35.035	65.450	13.032	1.00	17.81
ATOM	4208	N	GLY	B	310	34.475	63.900	11.485	1.00	18.08
ATOM	4209	CA	GLY	B	310	35.425	62.907	11.924	1.00	20.86
ATOM	4210	C	GLY	B	310	34.756	61.575	11.705	1.00	22.42
ATOM	4211	O	GLY	B	310	34.030	61.400	10.725	1.00	23.61
ATOM	4212	N	THR	B	311	35.003	60.641	12.613	1.00	22.53
ATOM	4213	CA	THR	B	311	34.352	59.342	12.585	1.00	21.84
ATOM	4214	CB	THR	B	311	35.352	58.275	12.150	1.00	23.59
ATOM	4215	OG1	THR	B	311	35.755	58.539	10.800	1.00	24.41
ATOM	4216	CG2	THR	B	311	34.685	56.919	12.048	1.00	24.94
ATOM	4217	C	THR	B	311	33.857	59.110	14.000	1.00	21.08
ATOM	4218	O	THR	B	311	34.608	59.335	14.950	1.00	23.66
ATOM	4219	N	PRO	B	312	32.594	58.704	14.151	1.00	19.37
ATOM	4220	CA	PRO	B	312	31.945	58.698	15.467	1.00	17.05
ATOM	4221	CB	PRO	B	312	30.672	57.870	15.240	1.00	16.77
ATOM	4222	CG	PRO	B	312	30.808	57.292	13.879	1.00	19.01
ATOM	4223	CD	PRO	B	312	31.682	58.231	13.098	1.00	19.81
ATOM	4224	C	PRO	B	312	32.820	58.117	16.583	1.00	15.80
ATOM	4225	O	PRO	B	312	33.066	58.840	17.544	1.00	16.07
ATOM	4226	N	GLU	B	313	33.319	56.891	16.435	1.00	11.78
ATOM	4227	CA	GLU	B	313	34.069	56.226	17.496	1.00	10.83
ATOM	4228	CB	GLU	B	313	34.235	54.752	17.166	1.00	17.06
ATOM	4229	CG	GLU	B	313	32.925	54.014	16.950	1.00	25.85
ATOM	4230	CD	GLU	B	313	32.535	53.899	15.485	1.00	28.53
ATOM	4231	OE1	GLU	B	313	32.964	54.764	14.693	1.00	29.32
ATOM	4232	OE2	GLU	B	313	31.790	52.947	15.132	1.00	31.09
ATOM	4233	C	GLU	B	313	35.437	56.835	17.801	1.00	10.32
ATOM	4234	O	GLU	B	313	36.081	56.458	18.771	1.00	8.56
ATOM	4235	N	TYR	B	314	35.876	57.781	16.980	1.00	12.37
ATOM	4236	CA	TYR	B	314	37.155	58.465	17.197	1.00	14.09
ATOM	4237	CB	TYR	B	314	38.044	58.356	15.947	1.00	12.21
ATOM	4238	CG	TYR	B	314	38.491	56.961	15.583	1.00	11.23
ATOM	4239	CD1	TYR	B	314	37.640	56.081	14.924	1.00	12.44
ATOM	4240	CE1	TYR	B	314	38.063	54.800	14.570	1.00	13.78
ATOM	4241	CZ	TYR	B	314	39.354	54.388	14.879	1.00	14.18

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4242	OH	TYR	B	314	39.786	53.116	14.528	1.00	15.73
ATOM	4243	CE2	TYR	B	314	40.215	55.256	15.519	1.00	13.25
ATOM	4244	CD2	TYR	B	314	39.782	56.536	15.859	1.00	12.61
ATOM	4245	C	TYR	B	314	37.039	59.950	17.610	1.00	14.42
ATOM	4246	O	TYR	B	314	38.039	60.564	17.960	1.00	17.54
ATOM	4247	N	LEU	B	315	35.844	60.531	17.546	1.00	13.41
ATOM	4248	CA	LEU	B	315	35.651	61.942	17.904	1.00	15.02
ATOM	4249	CB	LEU	B	315	34.181	62.331	17.777	1.00	13.22
ATOM	4250	CG	LEU	B	315	33.465	62.203	16.442	1.00	11.72
ATOM	4251	CD1	LEU	B	315	32.011	62.568	16.657	1.00	13.04
ATOM	4252	CD2	LEU	B	315	34.079	63.107	15.397	1.00	11.32
ATOM	4253	C	LEU	B	315	36.115	62.305	19.318	1.00	16.92
ATOM	4254	O	LEU	B	315	35.769	61.635	20.290	1.00	24.05
ATOM	4255	N	ALA	B	316	36.884	63.379	19.431	1.00	15.91
ATOM	4256	CA	ALA	B	316	37.336	63.860	20.736	1.00	13.63
ATOM	4257	CB	ALA	B	316	38.520	64.778	20.569	1.00	18.24
ATOM	4258	C	ALA	B	316	36.218	64.593	21.458	1.00	10.27
ATOM	4259	O	ALA	B	316	35.422	65.282	20.835	1.00	9.45
ATOM	4260	N	PRO	B	317	36.160	64.447	22.773	1.00	7.68
ATOM	4261	CA	PRO	B	317	35.129	65.088	23.589	1.00	6.85
ATOM	4262	CB	PRO	B	317	35.786	65.107	24.968	1.00	5.83
ATOM	4263	CG	PRO	B	317	36.494	63.810	25.004	1.00	5.99
ATOM	4264	CD	PRO	B	317	37.051	63.619	23.602	1.00	8.16
ATOM	4265	C	PRO	B	317	34.709	66.494	23.148	1.00	7.55
ATOM	4266	O	PRO	B	317	33.518	66.797	23.125	1.00	9.06
ATOM	4267	N	GLU	B	318	35.671	67.331	22.790	1.00	9.59
ATOM	4268	CA	GLU	B	318	35.407	68.735	22.491	1.00	8.77
ATOM	4269	CB	GLU	B	318	36.685	69.557	22.670	1.00	9.97
ATOM	4270	CG	GLU	B	318	37.744	69.279	21.616	1.00	13.10
ATOM	4271	CD	GLU	B	318	38.691	68.154	21.987	1.00	15.50
ATOM	4272	OE1	GLU	B	318	38.287	67.204	22.693	1.00	18.20
ATOM	4273	OE2	GLU	B	318	39.859	68.219	21.563	1.00	18.63
ATOM	4274	C	GLU	B	318	34.794	68.949	21.100	1.00	8.79
ATOM	4275	O	GLU	B	318	34.173	69.968	20.844	1.00	13.25
ATOM	4276	N	VAL	B	319	34.965	67.989	20.203	1.00	8.20
ATOM	4277	CA	VAL	B	319	34.271	68.007	18.921	1.00	6.16
ATOM	4278	CB	VAL	B	319	34.911	67.000	17.951	1.00	8.45
ATOM	4279	CG1	VAL	B	319	34.131	66.891	16.651	1.00	10.62
ATOM	4280	CG2	VAL	B	319	36.346	67.392	17.670	1.00	9.41
ATOM	4281	C	VAL	B	319	32.776	67.709	19.126	1.00	6.05
ATOM	4282	O	VAL	B	319	31.955	68.019	18.266	1.00	6.41
ATOM	4283	N	LEU	B	320	32.434	67.124	20.274	1.00	5.83
ATOM	4284	CA	LEU	B	320	31.042	66.902	20.662	1.00	8.71
ATOM	4285	CB	LEU	B	320	30.870	65.509	21.274	1.00	2.79
ATOM	4286	CG	LEU	B	320	31.159	64.281	20.416	1.00	2.34
ATOM	4287	CD1	LEU	B	320	31.272	63.091	21.304	1.00	3.00
ATOM	4288	CD2	LEU	B	320	30.097	64.025	19.351	1.00	2.90
ATOM	4289	C	LEU	B	320	30.519	67.971	21.638	1.00	15.55
ATOM	4290	O	LEU	B	320	29.320	68.021	21.950	1.00	16.84
ATOM	4291	N	GLU	B	321	31.422	68.835	22.094	1.00	22.42
ATOM	4292	CA	GLU	B	321	31.134	69.770	23.173	1.00	29.74
ATOM	4293	CB	GLU	B	321	31.607	69.153	24.484	1.00	31.35

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4294	CG	GLU	B	321	30.506	68.427	25.219	1.00	37.27
ATOM	4295	CD	GLU	B	321	29.942	69.265	26.344	1.00	42.49
ATOM	4296	OE1	GLU	B	321	30.754	69.695	27.198	1.00	45.23
ATOM	4297	OE2	GLU	B	321	28.704	69.500	26.373	1.00	42.64
ATOM	4298	C	GLU	B	321	31.757	71.166	22.961	1.00	34.59
ATOM	4299	O	GLU	B	321	32.983	71.326	22.919	1.00	37.16
ATOM	4300	N	ASP	B	322	30.903	72.180	22.853	1.00	37.44
ATOM	4301	CA	ASP	B	322	31.328	73.535	22.470	1.00	40.65
ATOM	4302	CB	ASP	B	322	32.434	74.099	23.389	1.00	41.61
ATOM	4303	CG	ASP	B	322	32.130	75.525	23.879	1.00	42.71
ATOM	4304	OD1	ASP	B	322	32.293	75.783	25.093	1.00	42.32
ATOM	4305	OD2	ASP	B	322	31.729	76.450	23.129	1.00	41.67
ATOM	4306	C	ASP	B	322	31.730	73.613	20.989	1.00	40.63
ATOM	4307	O	ASP	B	322	32.306	72.666	20.425	1.00	38.23
ATOM	4308	N	ASN	B	323	31.423	74.761	20.379	1.00	39.51
ATOM	4309	CA	ASN	B	323	31.488	74.928	18.925	1.00	37.84
ATOM	4310	CB	ASN	B	323	30.424	75.925	18.436	1.00	36.86
ATOM	4311	CG	ASN	B	323	29.498	76.400	19.548	1.00	37.44
ATOM	4312	OD1	ASN	B	323	29.400	77.599	19.811	1.00	38.17
ATOM	4313	ND2	ASN	B	323	28.806	75.464	20.195	1.00	36.47
ATOM	4314	C	ASN	B	323	32.875	75.285	18.374	1.00	36.80
ATOM	4315	O	ASN	B	323	32.981	75.908	17.309	1.00	37.57
ATOM	4316	N	ASP	B	324	33.927	74.871	19.088	1.00	33.06
ATOM	4317	CA	ASP	B	324	35.310	75.170	18.710	1.00	28.72
ATOM	4318	CB	ASP	B	324	35.715	76.549	19.232	1.00	31.13
ATOM	4319	CG	ASP	B	324	35.333	76.753	20.692	1.00	34.59
ATOM	4320	OD1	ASP	B	324	34.356	77.493	20.960	1.00	36.64
ATOM	4321	OD2	ASP	B	324	35.947	76.207	21.637	1.00	34.29
ATOM	4322	C	ASP	B	324	36.273	74.118	19.249	1.00	24.49
ATOM	4323	O	ASP	B	324	36.165	73.703	20.397	1.00	24.39
ATOM	4324	N	TYR	B	325	37.213	73.689	18.416	1.00	20.24
ATOM	4325	CA	TYR	B	325	38.232	72.740	18.836	1.00	17.31
ATOM	4326	CB	TYR	B	325	37.781	71.306	18.600	1.00	14.75
ATOM	4327	CG	TYR	B	325	37.466	70.927	17.162	1.00	14.79
ATOM	4328	CD1	TYR	B	325	38.457	70.459	16.296	1.00	13.00
ATOM	4329	CE1	TYR	B	325	38.154	70.076	14.990	1.00	11.33
ATOM	4330	CZ	TYR	B	325	36.846	70.157	14.544	1.00	13.15
ATOM	4331	OH	TYR	B	325	36.516	69.796	13.263	1.00	14.91
ATOM	4332	CE2	TYR	B	325	35.848	70.609	15.379	1.00	14.41
ATOM	4333	CD2	TYR	B	325	36.160	70.984	16.684	1.00	16.48
ATOM	4334	C	TYR	B	325	39.561	72.982	18.151	1.00	19.20
ATOM	4335	O	TYR	B	325	39.608	73.477	17.027	1.00	19.57
ATOM	4336	N	GLY	B	326	40.637	72.604	18.835	1.00	21.72
ATOM	4337	CA	GLY	B	326	41.986	72.881	18.375	1.00	21.26
ATOM	4338	C	GLY	B	326	42.671	71.717	17.690	1.00	20.47
ATOM	4339	O	GLY	B	326	42.047	70.708	17.356	1.00	17.47
ATOM	4340	N	ARG	B	327	43.973	71.869	17.477	1.00	20.74
ATOM	4341	CA	ARG	B	327	44.757	70.855	16.790	1.00	21.31
ATOM	4342	CB	ARG	B	327	46.113	71.423	16.379	1.00	23.72
ATOM	4343	CG	ARG	B	327	47.076	71.692	17.522	1.00	25.99
ATOM	4344	CD	ARG	B	327	48.529	71.470	17.131	1.00	28.60
ATOM	4345	NE	ARG	B	327	49.411	72.567	17.530	1.00	30.02

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4346	CZ	ARG	B	327	49.394	73.793	17.011	1.00	30.86
ATOM	4347	NH1	ARG	B	327	48.528	74.131	16.056	1.00	31.23
ATOM	4348	NH2	ARG	B	327	50.250	74.696	17.460	1.00	31.52
ATOM	4349	C	ARG	B	327	44.937	69.639	17.681	1.00	21.21
ATOM	4350	O	ARG	B	327	45.363	68.578	17.233	1.00	23.48
ATOM	4351	N	ALA	B	328	44.591	69.807	18.950	1.00	19.99
ATOM	4352	CA	ALA	B	328	44.769	68.775	19.953	1.00	17.18
ATOM	4353	CB	ALA	B	328	44.415	69.336	21.306	1.00	20.38
ATOM	4354	C	ALA	B	328	43.934	67.536	19.650	1.00	15.73
ATOM	4355	O	ALA	B	328	44.257	66.439	20.093	1.00	14.96
ATOM	4356	N	VAL	B	329	42.868	67.724	18.879	1.00	16.23
ATOM	4357	CA	VAL	B	329	41.957	66.641	18.495	1.00	16.29
ATOM	4358	CB	VAL	B	329	40.745	67.162	17.657	1.00	16.98
ATOM	4359	CG1	VAL	B	329	40.216	68.462	18.227	1.00	17.33
ATOM	4360	CG2	VAL	B	329	41.102	67.317	16.175	1.00	14.80
ATOM	4361	C	VAL	B	329	42.654	65.523	17.730	1.00	14.37
ATOM	4362	O	VAL	B	329	42.164	64.396	17.685	1.00	13.77
ATOM	4363	N	ASP	B	330	43.786	65.859	17.122	1.00	14.35
ATOM	4364	CA	ASP	B	330	44.592	64.902	16.393	1.00	14.73
ATOM	4365	CB	ASP	B	330	45.615	65.635	15.522	1.00	15.49
ATOM	4366	CG	ASP	B	330	45.235	65.642	14.045	1.00	15.11
ATOM	4367	OD1	ASP	B	330	44.370	64.825	13.644	1.00	14.60
ATOM	4368	OD2	ASP	B	330	45.759	66.424	13.218	1.00	12.82
ATOM	4369	C	ASP	B	330	45.278	63.942	17.369	1.00	14.54
ATOM	4370	O	ASP	B	330	45.361	62.738	17.112	1.00	11.53
ATOM	4371	N	TRP	B	331	45.744	64.470	18.498	1.00	16.03
ATOM	4372	CA	TRP	B	331	46.370	63.634	19.526	1.00	16.64
ATOM	4373	CB	TRP	B	331	47.178	64.474	20.505	1.00	19.05
ATOM	4374	CG	TRP	B	331	48.239	65.261	19.819	1.00	21.93
ATOM	4375	CD1	TRP	B	331	48.493	66.578	19.977	1.00	20.70
ATOM	4376	NE1	TRP	B	331	49.538	66.954	19.170	1.00	24.97
ATOM	4377	CE2	TRP	B	331	49.978	65.865	18.464	1.00	25.95
ATOM	4378	CD2	TRP	B	331	49.183	64.777	18.847	1.00	24.32
ATOM	4379	CE3	TRP	B	331	49.445	63.524	18.270	1.00	26.14
ATOM	4380	CZ3	TRP	B	331	50.475	63.410	17.338	1.00	25.95
ATOM	4381	CH2	TRP	B	331	51.242	64.511	16.980	1.00	27.19
ATOM	4382	CZ2	TRP	B	331	51.012	65.748	17.527	1.00	28.48
ATOM	4383	C	TRP	B	331	45.381	62.761	20.269	1.00	16.30
ATOM	4384	O	TRP	B	331	45.772	61.710	20.798	1.00	15.84
ATOM	4385	N	TRP	B	332	44.113	63.201	20.304	1.00	15.15
ATOM	4386	CA	TRP	B	332	43.020	62.388	20.826	1.00	11.35
ATOM	4387	CB	TRP	B	332	41.688	63.141	20.890	1.00	8.48
ATOM	4388	CG	TRP	B	332	40.585	62.189	21.238	1.00	10.41
ATOM	4389	CD1	TRP	B	332	39.854	61.432	20.372	1.00	12.65
ATOM	4390	NE1	TRP	B	332	38.965	60.636	21.057	1.00	15.47
ATOM	4391	CE2	TRP	B	332	39.125	60.849	22.402	1.00	14.32
ATOM	4392	CD2	TRP	B	332	40.140	61.823	22.555	1.00	12.86
ATOM	4393	CE3	TRP	B	332	40.495	62.219	23.857	1.00	10.28
ATOM	4394	CZ3	TRP	B	332	39.837	61.655	24.929	1.00	6.42
ATOM	4395	CH2	TRP	B	332	38.839	60.691	24.741	1.00	8.73
ATOM	4396	CZ2	TRP	B	332	38.467	60.274	23.492	1.00	11.29
ATOM	4397	C	TRP	B	332	42.881	61.180	19.920	1.00	12.52

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4398	O	TRP	B	332	42.926	60.038	20.380	1.00	14.93
ATOM	4399	N	GLY	B	333	42.727	61.445	18.627	1.00	12.63
ATOM	4400	CA	GLY	B	333	42.637	60.401	17.622	1.00	13.28
ATOM	4401	C	GLY	B	333	43.767	59.399	17.732	1.00	12.19
ATOM	4402	O	GLY	B	333	43.528	58.195	17.818	1.00	12.55
ATOM	4403	N	LEU	B	334	44.996	59.908	17.756	1.00	13.12
ATOM	4404	CA	LEU	B	334	46.190	59.076	17.876	1.00	13.17
ATOM	4405	CB	LEU	B	334	47.444	59.937	18.012	1.00	11.84
ATOM	4406	CG	LEU	B	334	48.625	59.104	18.486	1.00	12.18
ATOM	4407	CD1	LEU	B	334	49.242	58.340	17.335	1.00	12.00
ATOM	4408	CD2	LEU	B	334	49.640	59.960	19.186	1.00	15.03
ATOM	4409	C	LEU	B	334	46.091	58.120	19.054	1.00	13.54
ATOM	4410	O	LEU	B	334	46.466	56.949	18.944	1.00	16.15
ATOM	4411	N	GLY	B	335	45.576	58.623	20.172	1.00	11.75
ATOM	4412	CA	GLY	B	335	45.335	57.799	21.348	1.00	13.08
ATOM	4413	C	GLY	B	335	44.339	56.666	21.156	1.00	8.84
ATOM	4414	O	GLY	B	335	44.521	55.570	21.669	1.00	7.86
ATOM	4415	N	VAL	B	336	43.283	56.934	20.409	1.00	7.01
ATOM	4416	CA	VAL	B	336	42.305	55.909	20.115	1.00	6.97
ATOM	4417	CB	VAL	B	336	41.063	56.504	19.467	1.00	3.69
ATOM	4418	CG1	VAL	B	336	39.947	55.473	19.397	1.00	2.00
ATOM	4419	CG2	VAL	B	336	40.614	57.707	20.271	1.00	3.64
ATOM	4420	C	VAL	B	336	42.911	54.811	19.253	1.00	8.87
ATOM	4421	O	VAL	B	336	42.619	53.632	19.450	1.00	12.62
ATOM	4422	N	VAL	B	337	43.781	55.193	18.326	1.00	11.54
ATOM	4423	CA	VAL	B	337	44.434	54.224	17.440	1.00	14.78
ATOM	4424	CB	VAL	B	337	45.204	54.926	16.304	1.00	13.08
ATOM	4425	CG1	VAL	B	337	46.202	53.991	15.671	1.00	13.68
ATOM	4426	CG2	VAL	B	337	44.240	55.443	15.258	1.00	14.21
ATOM	4427	C	VAL	B	337	45.372	53.298	18.226	1.00	17.27
ATOM	4428	O	VAL	B	337	45.317	52.066	18.087	1.00	17.10
ATOM	4429	N	MET	B	338	46.215	53.899	19.059	1.00	16.78
ATOM	4430	CA	MET	B	338	47.142	53.147	19.892	1.00	16.49
ATOM	4431	CB	MET	B	338	48.058	54.108	20.634	1.00	18.95
ATOM	4432	CG	MET	B	338	48.762	55.066	19.737	1.00	20.97
ATOM	4433	SD	MET	B	338	50.500	54.742	19.695	1.00	24.33
ATOM	4434	CE	MET	B	338	51.093	56.371	20.031	1.00	23.99
ATOM	4435	C	MET	B	338	46.410	52.235	20.883	1.00	15.00
ATOM	4436	O	MET	B	338	46.736	51.057	20.986	1.00	14.57
ATOM	4437	N	TYR	B	339	45.424	52.787	21.596	1.00	12.04
ATOM	4438	CA	TYR	B	339	44.589	52.013	22.503	1.00	9.51
ATOM	4439	CB	TYR	B	339	43.369	52.816	22.961	1.00	10.12
ATOM	4440	CG	TYR	B	339	42.606	52.162	24.109	1.00	9.46
ATOM	4441	CD1	TYR	B	339	41.662	51.186	23.871	1.00	10.35
ATOM	4442	CE1	TYR	B	339	40.977	50.597	24.902	1.00	14.48
ATOM	4443	CZ	TYR	B	339	41.228	50.985	26.207	1.00	14.68
ATOM	4444	OH	TYR	B	339	40.541	50.383	27.249	1.00	17.45
ATOM	4445	CE2	TYR	B	339	42.160	51.959	26.468	1.00	9.71
ATOM	4446	CD2	TYR	B	339	42.835	52.538	25.430	1.00	9.10
ATOM	4447	C	TYR	B	339	44.098	50.778	21.796	1.00	11.30
ATOM	4448	O	TYR	B	339	44.179	49.671	22.338	1.00	10.56
ATOM	4449	N	GLU	B	340	43.570	50.984	20.589	1.00	11.24

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4450	CA	GLU	B	340	43.074	49.894	19.779	1.00	11.90
ATOM	4451	CB	GLU	B	340	42.558	50.409	18.447	1.00	13.52
ATOM	4452	CG	GLU	B	340	41.064	50.649	18.468	1.00	21.94
ATOM	4453	CD	GLU	B	340	40.530	51.261	17.181	1.00	28.56
ATOM	4454	OE1	GLU	B	340	40.818	52.461	16.914	1.00	29.69
ATOM	4455	OE2	GLU	B	340	39.798	50.544	16.448	1.00	30.78
ATOM	4456	C	GLU	B	340	44.176	48.873	19.585	1.00	12.55
ATOM	4457	O	GLU	B	340	43.979	47.705	19.870	1.00	11.29
ATOM	4458	N	MET	B	341	45.351	49.336	19.158	1.00	14.93
ATOM	4459	CA	MET	B	341	46.463	48.458	18.796	1.00	14.45
ATOM	4460	CB	MET	B	341	47.620	49.266	18.214	1.00	17.57
ATOM	4461	CG	MET	B	341	47.322	49.800	16.823	1.00	24.76
ATOM	4462	SD	MET	B	341	48.700	50.614	15.982	1.00	33.37
ATOM	4463	CE	MET	B	341	49.211	51.892	17.221	1.00	31.54
ATOM	4464	C	MET	B	341	46.937	47.631	19.964	1.00	12.78
ATOM	4465	O	MET	B	341	47.284	46.476	19.795	1.00	13.64
ATOM	4466	N	MET	B	342	46.919	48.223	21.151	1.00	14.31
ATOM	4467	CA	MET	B	342	47.476	47.595	22.339	1.00	14.71
ATOM	4468	CB	MET	B	342	48.242	48.619	23.171	1.00	15.87
ATOM	4469	CG	MET	B	342	49.612	48.942	22.614	1.00	20.88
ATOM	4470	SD	MET	B	342	50.417	50.389	23.361	1.00	26.64
ATOM	4471	CE	MET	B	342	50.144	51.676	22.133	1.00	23.62
ATOM	4472	C	MET	B	342	46.438	46.898	23.203	1.00	14.90
ATOM	4473	O	MET	B	342	46.805	46.079	24.039	1.00	18.91
ATOM	4474	N	CYS	B	343	45.158	47.210	23.014	1.00	13.67
ATOM	4475	CA	CYS	B	343	44.099	46.584	23.805	1.00	15.90
ATOM	4476	CB	CYS	B	343	43.246	47.629	24.506	1.00	19.25
ATOM	4477	SG	CYS	B	343	44.170	48.738	25.586	1.00	26.27
ATOM	4478	C	CYS	B	343	43.210	45.694	22.961	1.00	16.22
ATOM	4479	O	CYS	B	343	42.646	44.716	23.449	1.00	17.19
ATOM	4480	N	GLY	B	344	43.069	46.039	21.693	1.00	17.83
ATOM	4481	CA	GLY	B	344	42.328	45.199	20.774	1.00	20.58
ATOM	4482	C	GLY	B	344	40.860	45.542	20.698	1.00	20.75
ATOM	4483	O	GLY	B	344	40.069	44.743	20.208	1.00	23.39
ATOM	4484	N	ARG	B	345	40.506	46.732	21.180	1.00	20.83
ATOM	4485	CA	ARG	B	345	39.122	47.199	21.242	1.00	20.70
ATOM	4486	CB	ARG	B	345	38.356	46.513	22.397	1.00	25.58
ATOM	4487	CG	ARG	B	345	38.384	47.254	23.749	1.00	34.42
ATOM	4488	CD	ARG	B	345	37.400	46.749	24.845	1.00	41.97
ATOM	4489	NE	ARG	B	345	36.058	46.369	24.369	1.00	49.37
ATOM	4490	CZ	ARG	B	345	35.010	47.192	24.246	1.00	50.51
ATOM	4491	NH1	ARG	B	345	35.110	48.486	24.546	1.00	48.34
ATOM	4492	NH2	ARG	B	345	33.855	46.709	23.799	1.00	50.95
ATOM	4493	C	ARG	B	345	39.172	48.709	21.409	1.00	16.65
ATOM	4494	O	ARG	B	345	40.211	49.238	21.766	1.00	16.96
ATOM	4495	N	LEU	B	346	38.072	49.405	21.137	1.00	15.86
ATOM	4496	CA	LEU	B	346	38.032	50.862	21.315	1.00	14.17
ATOM	4497	CB	LEU	B	346	36.859	51.477	20.553	1.00	12.87
ATOM	4498	CG	LEU	B	346	36.834	51.339	19.031	1.00	15.21
ATOM	4499	CD1	LEU	B	346	35.403	51.358	18.490	1.00	13.86
ATOM	4500	CD2	LEU	B	346	37.662	52.438	18.390	1.00	15.93
ATOM	4501	C	LEU	B	346	37.925	51.248	22.787	1.00	13.00

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4502	O	LEU	B	346	37.323	50.528	23.579	1.00	16.80
ATOM	4503	N	PRO	B	347	38.490	52.388	23.150	1.00	9.96
ATOM	4504	CA	PRO	B	347	38.318	52.940	24.499	1.00	11.39
ATOM	4505	CB	PRO	B	347	38.877	54.354	24.368	1.00	12.35
ATOM	4506	CG	PRO	B	347	38.956	54.594	22.852	1.00	12.98
ATOM	4507	CD	PRO	B	347	39.310	53.255	22.292	1.00	10.27
ATOM	4508	C	PRO	B	347	36.844	53.030	24.848	1.00	13.11
ATOM	4509	O	PRO	B	347	36.444	52.736	25.975	1.00	19.49
ATOM	4510	N	PHE	B	348	36.038	53.447	23.881	1.00	10.96
ATOM	4511	CA	PHE	B	348	34.601	53.523	24.067	1.00	10.59
ATOM	4512	CB	PHE	B	348	34.172	54.956	24.345	1.00	8.94
ATOM	4513	CG	PHE	B	348	35.185	55.751	25.091	1.00	8.20
ATOM	4514	CD1	PHE	B	348	35.200	55.745	26.492	1.00	8.19
ATOM	4515	CE1	PHE	B	348	36.147	56.488	27.212	1.00	3.43
ATOM	4516	CZ	PHE	B	348	37.083	57.231	26.527	1.00	6.33
ATOM	4517	CE2	PHE	B	348	37.075	57.240	25.106	1.00	8.52
ATOM	4518	CD2	PHE	B	348	36.132	56.501	24.407	1.00	6.05
ATOM	4519	C	PHE	B	348	33.897	52.997	22.827	1.00	11.72
ATOM	4520	O	PHE	B	348	34.343	53.240	21.700	1.00	9.50
ATOM	4521	N	TYR	B	349	32.806	52.263	23.036	1.00	12.19
ATOM	4522	CA	TYR	B	349	32.048	51.724	21.922	1.00	14.74
ATOM	4523	CB	TYR	B	349	32.625	50.403	21.414	1.00	17.05
ATOM	4524	CG	TYR	B	349	31.803	49.839	20.286	1.00	19.31
ATOM	4525	CD1	TYR	B	349	31.926	50.339	18.978	1.00	18.91
ATOM	4526	CE1	TYR	B	349	31.154	49.837	17.940	1.00	20.17
ATOM	4527	CZ	TYR	B	349	30.230	48.829	18.216	1.00	24.26
ATOM	4528	OH	TYR	B	349	29.431	48.296	17.226	1.00	27.02
ATOM	4529	CE2	TYR	B	349	30.087	48.332	19.505	1.00	25.00
ATOM	4530	CD2	TYR	B	349	30.872	48.839	20.530	1.00	21.89
ATOM	4531	C	TYR	B	349	30.593	51.506	22.229	1.00	16.51
ATOM	4532	O	TYR	B	349	30.246	50.827	23.197	1.00	21.93
ATOM	4533	N	ASN	B	350	29.749	52.081	21.380	1.00	14.72
ATOM	4534	CA	ASN	B	350	28.396	51.587	21.203	1.00	10.73
ATOM	4535	CB	ASN	B	350	27.354	52.415	21.954	1.00	8.13
ATOM	4536	CG	ASN	B	350	26.196	51.559	22.455	1.00	7.47
ATOM	4537	OD1	ASN	B	350	25.112	52.048	22.687	1.00	8.42
ATOM	4538	ND2	ASN	B	350	26.436	50.269	22.622	1.00	7.62
ATOM	4539	C	ASN	B	350	28.052	51.508	19.741	1.00	9.35
ATOM	4540	O	ASN	B	350	28.652	52.195	18.917	1.00	12.88
ATOM	4541	N	GLN	B	351	27.107	50.635	19.424	1.00	8.29
ATOM	4542	CA	GLN	B	351	26.494	50.611	18.112	1.00	6.68
ATOM	4543	CB	GLN	B	351	25.756	49.303	17.912	1.00	4.08
ATOM	4544	CG	GLN	B	351	24.810	48.977	19.030	1.00	3.89
ATOM	4545	CD	GLN	B	351	25.262	47.789	19.822	1.00	9.19
ATOM	4546	OE1	GLN	B	351	26.462	47.553	19.966	1.00	13.80
ATOM	4547	NE2	GLN	B	351	24.308	47.026	20.342	1.00	11.36
ATOM	4548	C	GLN	B	351	25.516	51.771	18.046	1.00	7.52
ATOM	4549	O	GLN	B	351	25.179	52.264	16.961	1.00	7.56
ATOM	4550	N	ASP	B	352	25.051	52.195	19.218	1.00	6.61
ATOM	4551	CA	ASP	B	352	24.173	53.335	19.299	1.00	9.50
ATOM	4552	CB	ASP	B	352	23.289	53.259	20.536	1.00	11.10
ATOM	4553	CG	ASP	B	352	22.119	54.201	20.464	1.00	13.77

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4554	OD1	ASP	B	352	22.331	55.377	20.104	1.00	16.69
ATOM	4555	OD2	ASP	B	352	20.949	53.856	20.730	1.00	14.97
ATOM	4556	C	ASP	B	352	25.045	54.559	19.345	1.00	12.58
ATOM	4557	O	ASP	B	352	25.754	54.791	20.322	1.00	15.52
ATOM	4558	N	HIS	B	353	25.005	55.337	18.271	1.00	16.44
ATOM	4559	CA	HIS	B	353	25.826	56.536	18.168	1.00	17.21
ATOM	4560	CB	HIS	B	353	25.611	57.218	16.808	1.00	17.29
ATOM	4561	CG	HIS	B	353	26.403	56.619	15.686	1.00	17.09
ATOM	4562	ND1	HIS	B	353	26.140	56.899	14.363	1.00	16.55
ATOM	4563	CE1	HIS	B	353	26.996	56.247	13.594	1.00	18.31
ATOM	4564	NE2	HIS	B	353	27.806	55.551	14.371	1.00	19.70
ATOM	4565	CD2	HIS	B	353	27.460	55.769	15.685	1.00	20.09
ATOM	4566	C	HIS	B	353	25.519	57.505	19.321	1.00	17.84
ATOM	4567	O	HIS	B	353	26.379	58.271	19.733	1.00	18.70
ATOM	4568	N	GLU	B	354	24.299	57.464	19.850	1.00	19.74
ATOM	4569	CA	GLU	B	354	23.924	58.387	20.922	1.00	21.64
ATOM	4570	CB	GLU	B	354	22.413	58.534	21.047	1.00	25.66
ATOM	4571	CG	GLU	B	354	21.976	59.977	21.223	1.00	31.74
ATOM	4572	CD	GLU	B	354	20.700	60.097	22.028	1.00	36.15
ATOM	4573	OE1	GLU	B	354	19.634	59.685	21.517	1.00	38.49
ATOM	4574	OE2	GLU	B	354	20.762	60.601	23.172	1.00	38.35
ATOM	4575	C	GLU	B	354	24.521	58.002	22.258	1.00	18.94
ATOM	4576	O	GLU	B	354	24.861	58.877	23.057	1.00	18.67
ATOM	4577	N	LYS	B	355	24.639	56.693	22.488	1.00	15.94
ATOM	4578	CA	LYS	B	355	25.325	56.160	23.666	1.00	12.64
ATOM	4579	CB	LYS	B	355	24.972	54.693	23.910	1.00	12.00
ATOM	4580	CG	LYS	B	355	23.482	54.416	24.082	1.00	13.23
ATOM	4581	CD	LYS	B	355	23.238	53.296	25.082	1.00	12.88
ATOM	4582	CE	LYS	B	355	21.773	52.947	25.162	1.00	14.30
ATOM	4583	NZ	LYS	B	355	20.897	54.166	25.168	1.00	18.50
ATOM	4584	C	LYS	B	355	26.831	56.312	23.530	1.00	10.38
ATOM	4585	O	LYS	B	355	27.497	56.748	24.471	1.00	11.67
ATOM	4586	N	LEU	B	356	27.367	55.964	22.361	1.00	7.01
ATOM	4587	CA	LEU	B	356	28.799	56.108	22.107	1.00	6.20
ATOM	4588	CB	LEU	B	356	29.118	55.777	20.659	1.00	3.91
ATOM	4589	CG	LEU	B	356	30.481	56.212	20.142	1.00	3.82
ATOM	4590	CD1	LEU	B	356	31.558	55.270	20.631	1.00	3.20
ATOM	4591	CD2	LEU	B	356	30.459	56.251	18.640	1.00	5.15
ATOM	4592	C	LEU	B	356	29.334	57.500	22.489	1.00	8.29
ATOM	4593	O	LEU	B	356	30.388	57.622	23.121	1.00	10.05
ATOM	4594	N	PHE	B	357	28.591	58.536	22.119	1.00	9.67
ATOM	4595	CA	PHE	B	357	28.896	59.900	22.530	1.00	11.05
ATOM	4596	CB	PHE	B	357	28.038	60.895	21.766	1.00	8.33
ATOM	4597	CG	PHE	B	357	28.314	60.894	20.312	1.00	6.93
ATOM	4598	CD1	PHE	B	357	27.342	61.274	19.405	1.00	2.51
ATOM	4599	CE1	PHE	B	357	27.601	61.259	18.037	1.00	2.00
ATOM	4600	CZ	PHE	B	357	28.840	60.860	17.562	1.00	2.83
ATOM	4601	CE2	PHE	B	357	29.825	60.466	18.460	1.00	9.60
ATOM	4602	CD2	PHE	B	357	29.558	60.474	19.836	1.00	8.40
ATOM	4603	C	PHE	B	357	28.782	60.127	24.029	1.00	14.12
ATOM	4604	O	PHE	B	357	29.632	60.812	24.593	1.00	16.62
ATOM	4605	N	GLU	B	358	27.762	59.556	24.676	1.00	15.51

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4606	CA	GLU	B	358	27.695	59.586	26.145	1.00	20.01
ATOM	4607	CB	GLU	B	358	26.482	58.807	26.704	1.00	25.52
ATOM	4608	CG	GLU	B	358	26.433	58.673	28.230	1.00	34.33
ATOM	4609	CD	GLU	B	358	25.306	59.482	28.893	1.00	43.08
ATOM	4610	OE1	GLU	B	358	25.499	60.698	29.159	1.00	46.52
ATOM	4611	OE2	GLU	B	358	24.221	58.907	29.177	1.00	45.48
ATOM	4612	C	GLU	B	358	29.013	59.040	26.700	1.00	18.83
ATOM	4613	O	GLU	B	358	29.654	59.683	27.526	1.00	18.81
ATOM	4614	N	LEU	B	359	29.435	57.880	26.206	1.00	15.04
ATOM	4615	CA	LEU	B	359	30.674	57.283	26.658	1.00	12.45
ATOM	4616	CB	LEU	B	359	30.892	55.946	25.972	1.00	11.34
ATOM	4617	CG	LEU	B	359	29.887	54.846	26.281	1.00	9.03
ATOM	4618	CD1	LEU	B	359	30.314	53.574	25.557	1.00	8.31
ATOM	4619	CD2	LEU	B	359	29.799	54.621	27.766	1.00	9.77
ATOM	4620	C	LEU	B	359	31.879	58.210	26.458	1.00	14.30
ATOM	4621	O	LEU	B	359	32.547	58.549	27.437	1.00	14.39
ATOM	4622	N	ILE	B	360	32.140	58.634	25.213	1.00	13.76
ATOM	4623	CA	ILE	B	360	33.250	59.557	24.914	1.00	11.97
ATOM	4624	CB	ILE	B	360	33.255	60.031	23.426	1.00	8.94
ATOM	4625	CG1	ILE	B	360	33.975	59.010	22.561	1.00	10.03
ATOM	4626	CD1	ILE	B	360	33.231	58.611	21.354	1.00	9.82
ATOM	4627	CG2	ILE	B	360	33.990	61.364	23.251	1.00	2.23
ATOM	4628	C	ILE	B	360	33.328	60.750	25.872	1.00	14.69
ATOM	4629	O	ILE	B	360	34.425	61.081	26.316	1.00	19.53
ATOM	4630	N	LEU	B	361	32.194	61.381	26.199	1.00	10.03
ATOM	4631	CA	LEU	B	361	32.198	62.498	27.158	1.00	7.39
ATOM	4632	CB	LEU	B	361	31.152	63.556	26.806	1.00	8.80
ATOM	4633	CG	LEU	B	361	30.569	63.740	25.412	1.00	9.05
ATOM	4634	CD1	LEU	B	361	29.076	64.082	25.488	1.00	5.64
ATOM	4635	CD2	LEU	B	361	31.338	64.829	24.719	1.00	10.40
ATOM	4636	C	LEU	B	361	32.046	62.150	28.652	1.00	6.86
ATOM	4637	O	LEU	B	361	32.473	62.917	29.502	1.00	5.61
ATOM	4638	N	MET	B	362	31.447	61.012	28.979	1.00	9.11
ATOM	4639	CA	MET	B	362	31.179	60.689	30.386	1.00	13.18
ATOM	4640	CB	MET	B	362	29.692	60.362	30.616	1.00	19.25
ATOM	4641	CG	MET	B	362	28.734	61.501	30.348	1.00	21.48
ATOM	4642	SD	MET	B	362	29.268	62.998	31.149	1.00	26.74
ATOM	4643	CE	MET	B	362	29.231	64.193	29.771	1.00	28.98
ATOM	4644	C	MET	B	362	32.051	59.607	31.040	1.00	12.57
ATOM	4645	O	MET	B	362	32.486	59.793	32.182	1.00	10.93
ATOM	4646	N	GLU	B	363	32.269	58.478	30.354	1.00	13.09
ATOM	4647	CA	GLU	B	363	33.051	57.371	30.927	1.00	16.46
ATOM	4648	CB	GLU	B	363	32.879	56.050	30.164	1.00	20.77
ATOM	4649	CG	GLU	B	363	33.637	54.888	30.816	1.00	27.84
ATOM	4650	CD	GLU	B	363	33.685	53.621	29.967	1.00	34.76
ATOM	4651	OE1	GLU	B	363	34.755	53.331	29.373	1.00	38.61
ATOM	4652	OE2	GLU	B	363	32.659	52.898	29.898	1.00	37.60
ATOM	4653	C	GLU	B	363	34.517	57.719	30.955	1.00	15.96
ATOM	4654	O	GLU	B	363	35.063	58.213	29.976	1.00	18.32
ATOM	4655	N	GLU	B	364	35.167	57.461	32.076	1.00	16.91
ATOM	4656	CA	GLU	B	364	36.591	57.706	32.128	1.00	17.56
ATOM	4657	CB	GLU	B	364	37.032	58.251	33.479	1.00	19.72

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4658	CG	GLU	B	364	37.214	57.225	34.563	1.00	22.39
ATOM	4659	CD	GLU	B	364	38.290	57.662	35.515	1.00	28.14
ATOM	4660	OE1	GLU	B	364	37.954	58.422	36.462	1.00	29.82
ATOM	4661	OE2	GLU	B	364	39.465	57.267	35.289	1.00	29.69
ATOM	4662	C	GLU	B	364	37.306	56.434	31.744	1.00	15.21
ATOM	4663	O	GLU	B	364	36.823	55.330	32.008	1.00	14.26
ATOM	4664	N	ILE	B	365	38.450	56.621	31.095	1.00	14.13
ATOM	4665	CA	ILE	B	365	39.155	55.563	30.391	1.00	10.52
ATOM	4666	CB	ILE	B	365	40.318	56.166	29.578	1.00	8.59
ATOM	4667	CG1	ILE	B	365	41.045	55.081	28.793	1.00	11.25
ATOM	4668	CD1	ILE	B	365	40.713	55.089	27.299	1.00	14.08
ATOM	4669	CG2	ILE	B	365	41.260	56.968	30.456	1.00	12.05
ATOM	4670	C	ILE	B	365	39.593	54.414	31.297	1.00	12.16
ATOM	4671	O	ILE	B	365	39.985	54.617	32.456	1.00	14.78
ATOM	4672	N	ARG	B	366	39.469	53.202	30.768	1.00	9.13
ATOM	4673	CA	ARG	B	366	39.806	52.001	31.511	1.00	5.91
ATOM	4674	CB	ARG	B	366	38.569	51.141	31.728	1.00	6.72
ATOM	4675	CG	ARG	B	366	37.302	51.699	31.175	1.00	5.57
ATOM	4676	CD	ARG	B	366	36.192	51.744	32.196	1.00	7.28
ATOM	4677	NE	ARG	B	366	35.486	50.467	32.368	1.00	8.60
ATOM	4678	CZ	ARG	B	366	34.907	49.731	31.404	1.00	7.70
ATOM	4679	NH1	ARG	B	366	34.934	50.083	30.118	1.00	2.00
ATOM	4680	NH2	ARG	B	366	34.288	48.610	31.745	1.00	9.51
ATOM	4681	C	ARG	B	366	40.837	51.215	30.732	1.00	5.29
ATOM	4682	O	ARG	B	366	40.873	51.272	29.515	1.00	11.26
ATOM	4683	N	PHE	B	367	41.686	50.478	31.416	1.00	2.51
ATOM	4684	CA	PHE	B	367	42.754	49.811	30.712	1.00	2.34
ATOM	4685	CB	PHE	B	367	44.106	50.462	30.991	1.00	2.00
ATOM	4686	CG	PHE	B	367	44.214	51.848	30.478	1.00	2.00
ATOM	4687	CD1	PHE	B	367	44.468	52.081	29.148	1.00	2.00
ATOM	4688	CE1	PHE	B	367	44.546	53.385	28.662	1.00	4.02
ATOM	4689	CZ	PHE	B	367	44.374	54.462	29.522	1.00	2.28
ATOM	4690	CE2	PHE	B	367	44.116	54.229	30.855	1.00	2.00
ATOM	4691	CD2	PHE	B	367	44.041	52.929	31.325	1.00	2.00
ATOM	4692	C	PHE	B	367	42.768	48.426	31.227	1.00	5.34
ATOM	4693	O	PHE	B	367	42.487	48.215	32.399	1.00	7.97
ATOM	4694	N	PRO	B	368	43.078	47.478	30.351	1.00	5.96
ATOM	4695	CA	PRO	B	368	43.335	46.112	30.778	1.00	4.44
ATOM	4696	CB	PRO	B	368	43.612	45.374	29.472	1.00	2.39
ATOM	4697	CG	PRO	B	368	43.928	46.403	28.494	1.00	6.08
ATOM	4698	CD	PRO	B	368	43.208	47.644	28.895	1.00	7.37
ATOM	4699	C	PRO	B	368	44.566	46.145	31.663	1.00	7.59
ATOM	4700	O	PRO	B	368	45.464	46.958	31.426	1.00	6.91
ATOM	4701	N	ARG	B	369	44.581	45.294	32.689	1.00	10.71
ATOM	4702	CA	ARG	B	369	45.707	45.186	33.612	1.00	9.32
ATOM	4703	CB	ARG	B	369	45.340	44.264	34.772	1.00	7.65
ATOM	4704	CG	ARG	B	369	45.497	44.895	36.139	1.00	8.23
ATOM	4705	CD	ARG	B	369	44.554	44.322	37.165	1.00	7.83
ATOM	4706	NE	ARG	B	369	45.152	43.956	38.456	1.00	8.74
ATOM	4707	CZ	ARG	B	369	45.855	42.849	38.698	1.00	12.73
ATOM	4708	NH1	ARG	B	369	46.135	41.971	37.728	1.00	14.60
ATOM	4709	NH2	ARG	B	369	46.289	42.615	39.931	1.00	14.63

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4710	C	ARG	B	369	46.993	44.703	32.923	1.00	9.65
ATOM	4711	O	ARG	B	369	48.081	44.809	33.497	1.00	12.90
ATOM	4712	N	THR	B	370	46.859	44.209	31.692	1.00	7.86
ATOM	4713	CA	THR	B	370	47.973	43.637	30.940	1.00	8.09
ATOM	4714	CB	THR	B	370	47.504	42.487	29.984	1.00	9.51
ATOM	4715	OG1	THR	B	370	46.387	42.904	29.171	1.00	5.06
ATOM	4716	CG2	THR	B	370	46.999	41.280	30.799	1.00	10.09
ATOM	4717	C	THR	B	370	48.795	44.662	30.174	1.00	7.49
ATOM	4718	O	THR	B	370	49.795	44.313	29.555	1.00	11.12
ATOM	4719	N	LEU	B	371	48.382	45.920	30.207	1.00	5.89
ATOM	4720	CA	LEU	B	371	49.158	46.976	29.572	1.00	3.75
ATOM	4721	CB	LEU	B	371	48.312	48.244	29.414	1.00	2.08
ATOM	4722	CG	LEU	B	371	48.408	49.011	28.099	1.00	2.00
ATOM	4723	CD1	LEU	B	371	48.424	48.045	26.930	1.00	3.65
ATOM	4724	CD2	LEU	B	371	47.262	50.006	27.969	1.00	2.00
ATOM	4725	C	LEU	B	371	50.394	47.294	30.393	1.00	2.00
ATOM	4726	O	LEU	B	371	50.367	47.226	31.617	1.00	2.00
ATOM	4727	N	GLY	B	372	51.475	47.651	29.715	1.00	4.05
ATOM	4728	CA	GLY	B	372	52.622	48.248	30.382	1.00	10.07
ATOM	4729	C	GLY	B	372	52.296	49.531	31.155	1.00	10.20
ATOM	4730	O	GLY	B	372	51.306	50.198	30.849	1.00	11.60
ATOM	4731	N	PRO	B	373	53.101	49.859	32.170	1.00	8.83
ATOM	4732	CA	PRO	B	373	53.008	51.151	32.866	1.00	6.22
ATOM	4733	CB	PRO	B	373	54.124	51.065	33.904	1.00	9.46
ATOM	4734	CG	PRO	B	373	54.246	49.590	34.164	1.00	11.59
ATOM	4735	CD	PRO	B	373	54.118	48.985	32.786	1.00	10.95
ATOM	4736	C	PRO	B	373	53.198	52.369	31.980	1.00	4.47
ATOM	4737	O	PRO	B	373	52.409	53.293	32.116	1.00	2.95
ATOM	4738	N	GLU	B	374	54.188	52.379	31.094	1.00	8.26
ATOM	4739	CA	GLU	B	374	54.384	53.531	30.205	1.00	15.16
ATOM	4740	CB	GLU	B	374	55.856	53.696	29.779	1.00	19.85
ATOM	4741	CG	GLU	B	374	56.445	52.567	28.952	1.00	28.64
ATOM	4742	CD	GLU	B	374	56.644	51.299	29.761	1.00	35.84
ATOM	4743	OE1	GLU	B	374	55.647	50.533	29.884	1.00	38.81
ATOM	4744	OE2	GLU	B	374	57.779	51.072	30.274	1.00	37.08
ATOM	4745	C	GLU	B	374	53.417	53.566	29.006	1.00	17.35
ATOM	4746	O	GLU	B	374	53.197	54.617	28.395	1.00	17.20
ATOM	4747	N	ALA	B	375	52.827	52.419	28.678	1.00	19.32
ATOM	4748	CA	ALA	B	375	51.747	52.390	27.690	1.00	17.24
ATOM	4749	CB	ALA	B	375	51.422	50.967	27.302	1.00	17.75
ATOM	4750	C	ALA	B	375	50.527	53.078	28.280	1.00	14.03
ATOM	4751	O	ALA	B	375	50.039	54.083	27.745	1.00	10.60
ATOM	4752	N	LYS	B	376	50.062	52.526	29.400	1.00	13.22
ATOM	4753	CA	LYS	B	376	48.987	53.102	30.193	1.00	13.09
ATOM	4754	CB	LYS	B	376	48.994	52.491	31.588	1.00	11.06
ATOM	4755	CG	LYS	B	376	47.690	51.889	32.046	1.00	14.10
ATOM	4756	CD	LYS	B	376	47.913	50.530	32.781	1.00	20.14
ATOM	4757	CE	LYS	B	376	48.319	50.678	34.268	1.00	23.68
ATOM	4758	NZ	LYS	B	376	47.313	51.417	35.125	1.00	27.68
ATOM	4759	C	LYS	B	376	49.163	54.619	30.294	1.00	15.09
ATOM	4760	O	LYS	B	376	48.200	55.371	30.124	1.00	16.30
ATOM	4761	N	SER	B	377	50.393	55.067	30.551	1.00	12.63

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4762	CA	SER	B	377	50.630	56.484	30.777	1.00	12.31
ATOM	4763	CB	SER	B	377	51.964	56.739	31.470	1.00	13.61
ATOM	4764	OG	SER	B	377	52.032	58.090	31.891	1.00	16.33
ATOM	4765	C	SER	B	377	50.536	57.324	29.512	1.00	13.11
ATOM	4766	O	SER	B	377	50.140	58.483	29.585	1.00	17.27
ATOM	4767	N	LEU	B	378	50.904	56.766	28.361	1.00	10.26
ATOM	4768	CA	LEU	B	378	50.834	57.541	27.125	1.00	5.76
ATOM	4769	CB	LEU	B	378	51.666	56.915	26.016	1.00	3.43
ATOM	4770	CG	LEU	B	378	51.365	57.364	24.592	1.00	2.00
ATOM	4771	CD1	LEU	B	378	52.178	58.586	24.259	1.00	2.00
ATOM	4772	CD2	LEU	B	378	51.668	56.229	23.624	1.00	2.00
ATOM	4773	C	LEU	B	378	49.400	57.674	26.690	1.00	6.60
ATOM	4774	O	LEU	B	378	48.993	58.736	26.249	1.00	5.97
ATOM	4775	N	LEU	B	379	48.647	56.581	26.821	1.00	9.04
ATOM	4776	CA	LEU	B	379	47.233	56.552	26.465	1.00	9.66
ATOM	4777	CB	LEU	B	379	46.706	55.131	26.535	1.00	4.19
ATOM	4778	CG	LEU	B	379	47.225	54.242	25.418	1.00	5.73
ATOM	4779	CD1	LEU	B	379	46.522	52.896	25.475	1.00	6.27
ATOM	4780	CD2	LEU	B	379	47.040	54.891	24.058	1.00	2.59
ATOM	4781	C	LEU	B	379	46.410	57.464	27.368	1.00	12.95
ATOM	4782	O	LEU	B	379	45.664	58.311	26.889	1.00	13.92
ATOM	4783	N	SER	B	380	46.577	57.292	28.676	1.00	15.75
ATOM	4784	CA	SER	B	380	45.855	58.063	29.667	1.00	14.56
ATOM	4785	CB	SER	B	380	46.265	57.643	31.086	1.00	14.01
ATOM	4786	OG	SER	B	380	45.185	57.754	32.013	1.00	16.66
ATOM	4787	C	SER	B	380	46.121	59.535	29.436	1.00	15.10
ATOM	4788	O	SER	B	380	45.247	60.362	29.664	1.00	22.62
ATOM	4789	N	GLY	B	381	47.316	59.856	28.954	1.00	13.67
ATOM	4790	CA	GLY	B	381	47.686	61.236	28.677	1.00	14.15
ATOM	4791	C	GLY	B	381	47.106	61.752	27.371	1.00	12.27
ATOM	4792	O	GLY	B	381	46.678	62.892	27.301	1.00	10.44
ATOM	4793	N	LEU	B	382	47.100	60.902	26.342	1.00	13.78
ATOM	4794	CA	LEU	B	382	46.567	61.240	25.021	1.00	12.68
ATOM	4795	CB	LEU	B	382	46.985	60.191	23.994	1.00	8.24
ATOM	4796	CG	LEU	B	382	48.429	60.232	23.498	1.00	8.35
ATOM	4797	CD1	LEU	B	382	48.751	58.945	22.793	1.00	7.85
ATOM	4798	CD2	LEU	B	382	48.698	61.420	22.589	1.00	7.40
ATOM	4799	C	LEU	B	382	45.048	61.315	25.040	1.00	16.94
ATOM	4800	O	LEU	B	382	44.440	62.066	24.262	1.00	18.77
ATOM	4801	N	LEU	B	383	44.438	60.525	25.925	1.00	15.76
ATOM	4802	CA	LEU	B	383	42.989	60.442	26.003	1.00	10.53
ATOM	4803	CB	LEU	B	383	42.510	58.984	25.989	1.00	4.96
ATOM	4804	CG	LEU	B	383	42.782	58.220	24.688	1.00	4.47
ATOM	4805	CD1	LEU	B	383	42.371	56.776	24.794	1.00	3.93
ATOM	4806	CD2	LEU	B	383	42.075	58.855	23.509	1.00	7.12
ATOM	4807	C	LEU	B	383	42.427	61.232	27.174	1.00	12.02
ATOM	4808	O	LEU	B	383	41.405	60.865	27.757	1.00	18.13
ATOM	4809	N	LYS	B	384	43.079	62.338	27.508	1.00	12.50
ATOM	4810	CA	LYS	B	384	42.471	63.280	28.440	1.00	14.64
ATOM	4811	CB	LYS	B	384	43.492	64.277	28.988	1.00	13.39
ATOM	4812	CG	LYS	B	384	44.655	63.614	29.726	1.00	14.50
ATOM	4813	CD	LYS	B	384	44.620	63.850	31.223	1.00	14.30

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4814	CE	LYS	B	384	45.682	63.023	31.912	1.00	16.78
ATOM	4815	NZ	LYS	B	384	45.266	62.620	33.293	1.00	20.83
ATOM	4816	C	LYS	B	384	41.360	63.988	27.683	1.00	14.59
ATOM	4817	O	LYS	B	384	41.557	64.409	26.539	1.00	17.07
ATOM	4818	N	LYS	B	385	40.188	64.081	28.300	1.00	10.54
ATOM	4819	CA	LYS	B	385	39.030	64.653	27.627	1.00	8.68
ATOM	4820	CB	LYS	B	385	37.760	64.407	28.424	1.00	7.45
ATOM	4821	CG	LYS	B	385	37.541	62.968	28.768	1.00	6.96
ATOM	4822	CD	LYS	B	385	36.219	62.770	29.471	1.00	6.99
ATOM	4823	CE	LYS	B	385	35.535	61.488	29.002	1.00	7.08
ATOM	4824	NZ	LYS	B	385	36.465	60.334	28.757	1.00	12.14
ATOM	4825	C	LYS	B	385	39.192	66.136	27.373	1.00	10.15
ATOM	4826	O	LYS	B	385	38.705	66.646	26.368	1.00	11.63
ATOM	4827	N	ASP	B	386	39.865	66.820	28.294	1.00	13.93
ATOM	4828	CA	ASP	B	386	40.107	68.256	28.183	1.00	17.29
ATOM	4829	CB	ASP	B	386	40.223	68.908	29.567	1.00	20.29
ATOM	4830	CG	ASP	B	386	40.597	70.391	29.499	1.00	24.52
ATOM	4831	OD1	ASP	B	386	40.218	71.086	28.529	1.00	26.37
ATOM	4832	OD2	ASP	B	386	41.264	70.959	30.388	1.00	28.24
ATOM	4833	C	ASP	B	386	41.370	68.498	27.374	1.00	17.08
ATOM	4834	O	ASP	B	386	42.453	68.078	27.782	1.00	19.50
ATOM	4835	N	PRO	B	387	41.229	69.183	26.239	1.00	16.08
ATOM	4836	CA	PRO	B	387	42.343	69.409	25.310	1.00	16.17
ATOM	4837	CB	PRO	B	387	41.679	70.145	24.153	1.00	15.02
ATOM	4838	CG	PRO	B	387	40.237	69.897	24.320	1.00	15.37
ATOM	4839	CD	PRO	B	387	39.984	69.808	25.765	1.00	15.21
ATOM	4840	C	PRO	B	387	43.455	70.273	25.913	1.00	19.24
ATOM	4841	O	PRO	B	387	44.620	70.136	25.536	1.00	21.57
ATOM	4842	N	LYS	B	388	43.097	71.146	26.850	1.00	19.81
ATOM	4843	CA	LYS	B	388	44.083	71.940	27.576	1.00	19.31
ATOM	4844	CB	LYS	B	388	43.370	73.006	28.423	1.00	18.17
ATOM	4845	CG	LYS	B	388	43.081	74.312	27.659	1.00	17.80
ATOM	4846	CD	LYS	B	388	41.592	74.639	27.590	1.00	15.83
ATOM	4847	CE	LYS	B	388	41.261	75.859	28.447	1.00	14.50
ATOM	4848	NZ	LYS	B	388	40.561	76.927	27.686	1.00	11.38
ATOM	4849	C	LYS	B	388	45.017	71.061	28.435	1.00	19.41
ATOM	4850	O	LYS	B	388	46.099	71.496	28.832	1.00	20.21
ATOM	4851	N	GLN	B	389	44.601	69.815	28.672	1.00	18.15
ATOM	4852	CA	GLN	B	389	45.263	68.886	29.590	1.00	17.02
ATOM	4853	CB	GLN	B	389	44.245	68.447	30.641	1.00	18.88
ATOM	4854	CG	GLN	B	389	44.681	68.522	32.090	1.00	21.45
ATOM	4855	CD	GLN	B	389	43.571	68.045	33.041	1.00	24.71
ATOM	4856	OE1	GLN	B	389	43.223	66.850	33.082	1.00	24.94
ATOM	4857	NE2	GLN	B	389	43.016	68.978	33.803	1.00	25.49
ATOM	4858	C	GLN	B	389	45.808	67.642	28.861	1.00	15.29
ATOM	4859	O	GLN	B	389	46.562	66.846	29.431	1.00	15.31
ATOM	4860	N	ARG	B	390	45.421	67.487	27.601	1.00	11.99
ATOM	4861	CA	ARG	B	390	45.751	66.310	26.813	1.00	9.96
ATOM	4862	CB	ARG	B	390	44.740	66.169	25.665	1.00	9.74
ATOM	4863	CG	ARG	B	390	45.088	65.125	24.615	1.00	8.49
ATOM	4864	CD	ARG	B	390	44.015	64.894	23.545	1.00	11.21
ATOM	4865	NE	ARG	B	390	42.637	65.098	24.006	1.00	11.27

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4866	CZ	ARG	B	390	41.776	65.975	23.469	1.00	8.19
ATOM	4867	NH1	ARG	B	390	42.138	66.737	22.443	1.00	2.92
ATOM	4868	NH2	ARG	B	390	40.546	66.088	23.962	1.00	5.78
ATOM	4869	C	ARG	B	390	47.149	66.396	26.243	1.00	10.43
ATOM	4870	O	ARG	B	390	47.363	67.108	25.272	1.00	15.15
ATOM	4871	N	LEU	B	391	48.093	65.679	26.843	1.00	10.19
ATOM	4872	CA	LEU	B	391	49.427	65.465	26.259	1.00	13.75
ATOM	4873	CB	LEU	B	391	49.815	63.996	26.479	1.00	16.72
ATOM	4874	CG	LEU	B	391	51.137	63.373	26.021	1.00	18.33
ATOM	4875	CD1	LEU	B	391	52.191	63.456	27.101	1.00	20.44
ATOM	4876	CD2	LEU	B	391	50.897	61.932	25.685	1.00	18.53
ATOM	4877	C	LEU	B	391	49.516	65.840	24.760	1.00	14.90
ATOM	4878	O	LEU	B	391	49.199	65.037	23.900	1.00	14.10
ATOM	4879	N	GLY	B	392	49.927	67.070	24.462	1.00	18.54
ATOM	4880	CA	GLY	B	392	49.930	67.581	23.097	1.00	24.37
ATOM	4881	C	GLY	B	392	49.313	68.974	22.907	1.00	31.50
ATOM	4882	O	GLY	B	392	49.559	69.654	21.884	1.00	34.64
ATOM	4883	N	GLY	B	393	48.519	69.413	23.884	1.00	30.41
ATOM	4884	CA	GLY	B	393	47.796	70.666	23.770	1.00	32.56
ATOM	4885	C	GLY	B	393	48.485	71.868	24.398	1.00	36.15
ATOM	4886	O	GLY	B	393	47.810	72.783	24.898	1.00	38.26
ATOM	4887	N	GLY	B	394	49.819	71.874	24.382	1.00	34.80
ATOM	4888	CA	GLY	B	394	50.585	72.995	24.911	1.00	33.76
ATOM	4889	C	GLY	B	394	51.272	73.725	23.780	1.00	31.88
ATOM	4890	O	GLY	B	394	50.974	73.453	22.612	1.00	31.26
ATOM	4891	N	SER	B	395	52.181	74.645	24.107	1.00	28.79
ATOM	4892	CA	SER	B	395	53.032	75.239	23.082	1.00	27.08
ATOM	4893	CB	SER	B	395	54.147	76.067	23.715	1.00	25.22
ATOM	4894	OG	SER	B	395	53.618	77.146	24.455	1.00	26.24
ATOM	4895	C	SER	B	395	53.640	74.118	22.233	1.00	27.61
ATOM	4896	O	SER	B	395	53.434	74.049	21.018	1.00	23.10
ATOM	4897	N	GLU	B	396	54.327	73.211	22.925	1.00	30.57
ATOM	4898	CA	GLU	B	396	55.229	72.206	22.350	1.00	33.83
ATOM	4899	CB	GLU	B	396	55.884	71.416	23.494	1.00	37.99
ATOM	4900	CG	GLU	B	396	54.890	70.647	24.368	1.00	42.84
ATOM	4901	CD	GLU	B	396	55.072	70.859	25.869	1.00	44.81
ATOM	4902	OE1	GLU	B	396	56.219	70.772	26.373	1.00	45.53
ATOM	4903	OE2	GLU	B	396	54.049	71.091	26.554	1.00	46.06
ATOM	4904	C	GLU	B	396	54.671	71.243	21.279	1.00	33.27
ATOM	4905	O	GLU	B	396	55.419	70.797	20.406	1.00	31.56
ATOM	4906	N	ASP	B	397	53.381	70.908	21.360	1.00	34.54
ATOM	4907	CA	ASP	B	397	52.720	70.014	20.393	1.00	31.74
ATOM	4908	CB	ASP	B	397	52.781	70.602	18.971	1.00	33.35
ATOM	4909	CG	ASP	B	397	51.819	69.931	18.025	1.00	33.30
ATOM	4910	OD1	ASP	B	397	50.704	69.613	18.475	1.00	33.64
ATOM	4911	OD2	ASP	B	397	52.092	69.666	16.835	1.00	33.13
ATOM	4912	C	ASP	B	397	53.271	68.581	20.410	1.00	29.56
ATOM	4913	O	ASP	B	397	53.436	67.990	21.475	1.00	28.58
ATOM	4914	N	ALA	B	398	53.560	68.046	19.223	1.00	28.18
ATOM	4915	CA	ALA	B	398	54.031	66.676	19.033	1.00	25.89
ATOM	4916	CB	ALA	B	398	54.292	66.418	17.563	1.00	24.12
ATOM	4917	C	ALA	B	398	55.274	66.356	19.853	1.00	26.09

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4918	O	ALA	B	398	55.518	65.190	20.188	1.00	26.79
ATOM	4919	N	LYS	B	399	56.052	67.394	20.158	1.00	25.13
ATOM	4920	CA	LYS	B	399	57.205	67.296	21.048	1.00	26.19
ATOM	4921	CB	LYS	B	399	57.720	68.699	21.393	1.00	28.61
ATOM	4922	CG	LYS	B	399	59.237	68.870	21.379	1.00	30.31
ATOM	4923	CD	LYS	B	399	59.646	70.184	20.692	1.00	32.29
ATOM	4924	CE	LYS	B	399	59.984	71.289	21.704	1.00	33.00
ATOM	4925	NZ	LYS	B	399	60.789	72.398	21.105	1.00	29.82
ATOM	4926	C	LYS	B	399	56.836	66.547	22.332	1.00	25.79
ATOM	4927	O	LYS	B	399	57.478	65.554	22.683	1.00	25.48
ATOM	4928	N	GLU	B	400	55.785	67.026	23.006	1.00	25.55
ATOM	4929	CA	GLU	B	400	55.288	66.464	24.272	1.00	24.77
ATOM	4930	CB	GLU	B	400	53.938	67.106	24.653	1.00	26.39
ATOM	4931	CG	GLU	B	400	53.779	67.510	26.119	1.00	26.89
ATOM	4932	CD	GLU	B	400	52.510	68.318	26.383	1.00	28.74
ATOM	4933	OE1	GLU	B	400	52.146	69.188	25.554	1.00	28.39
ATOM	4934	OE2	GLU	B	400	51.868	68.083	27.429	1.00	29.74
ATOM	4935	C	GLU	B	400	55.137	64.944	24.207	1.00	22.68
ATOM	4936	O	GLU	B	400	55.404	64.251	25.193	1.00	22.99
ATOM	4937	N	ILE	B	401	54.712	64.451	23.040	1.00	17.70
ATOM	4938	CA	ILE	B	401	54.475	63.033	22.812	1.00	13.94
ATOM	4939	CB	ILE	B	401	53.459	62.847	21.666	1.00	14.15
ATOM	4940	CG1	ILE	B	401	52.048	62.898	22.224	1.00	14.04
ATOM	4941	CD1	ILE	B	401	51.276	64.043	21.696	1.00	18.56
ATOM	4942	CG2	ILE	B	401	53.648	61.526	20.929	1.00	13.92
ATOM	4943	C	ILE	B	401	55.769	62.280	22.544	1.00	12.44
ATOM	4944	O	ILE	B	401	55.936	61.143	22.985	1.00	11.72
ATOM	4945	N	MET	B	402	56.684	62.915	21.824	1.00	12.24
ATOM	4946	CA	MET	B	402	57.963	62.297	21.500	1.00	10.51
ATOM	4947	CB	MET	B	402	58.660	63.105	20.421	1.00	10.94
ATOM	4948	CG	MET	B	402	57.900	63.111	19.108	1.00	13.95
ATOM	4949	SD	MET	B	402	58.341	64.408	17.917	1.00	20.12
ATOM	4950	CE	MET	B	402	59.970	65.037	18.520	1.00	19.55
ATOM	4951	C	MET	B	402	58.841	62.146	22.740	1.00	10.46
ATOM	4952	O	MET	B	402	59.511	61.131	22.907	1.00	10.50
ATOM	4953	N	GLN	B	403	58.808	63.142	23.622	1.00	10.83
ATOM	4954	CA	GLN	B	403	59.545	63.088	24.884	1.00	13.29
ATOM	4955	CB	GLN	B	403	59.663	64.484	25.505	1.00	14.52
ATOM	4956	CG	GLN	B	403	60.672	65.434	24.871	1.00	14.98
ATOM	4957	CD	GLN	B	403	60.516	66.858	25.405	1.00	17.09
ATOM	4958	OE1	GLN	B	403	61.496	67.598	25.527	1.00	17.64
ATOM	4959	NE2	GLN	B	403	59.281	67.238	25.739	1.00	18.02
ATOM	4960	C	GLN	B	403	58.926	62.139	25.926	1.00	14.85
ATOM	4961	O	GLN	B	403	59.525	61.921	26.987	1.00	18.25
ATOM	4962	N	HIS	B	404	57.738	61.596	25.640	1.00	14.60
ATOM	4963	CA	HIS	B	404	57.031	60.689	26.560	1.00	12.42
ATOM	4964	CB	HIS	B	404	55.643	60.357	26.034	1.00	10.49
ATOM	4965	CG	HIS	B	404	54.775	59.698	27.049	1.00	11.74
ATOM	4966	ND1	HIS	B	404	54.853	58.353	27.328	1.00	12.95
ATOM	4967	CE1	HIS	B	404	53.992	58.051	28.283	1.00	12.88
ATOM	4968	NE2	HIS	B	404	53.361	59.154	28.638	1.00	13.64
ATOM	4969	CD2	HIS	B	404	53.835	60.200	27.882	1.00	14.30

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	4970	C	HIS	B	404	57.789	59.388	26.774	1.00	14.58
ATOM	4971	O	HIS	B	404	58.390	58.863	25.826	1.00	17.22
ATOM	4972	N	ARG	B	405	57.748	58.865	28.007	1.00	13.51
ATOM	4973	CA	ARG	B	405	58.546	57.683	28.391	1.00	10.40
ATOM	4974	CB	ARG	B	405	58.389	57.332	29.881	1.00	12.61
ATOM	4975	CG	ARG	B	405	57.022	57.631	30.492	1.00	20.03
ATOM	4976	CD	ARG	B	405	57.012	57.588	32.012	1.00	24.92
ATOM	4977	NE	ARG	B	405	55.825	56.948	32.594	1.00	28.15
ATOM	4978	CZ	ARG	B	405	55.850	55.860	33.379	1.00	31.85
ATOM	4979	NH1	ARG	B	405	57.002	55.249	33.675	1.00	33.78
ATOM	4980	NH2	ARG	B	405	54.714	55.376	33.878	1.00	30.85
ATOM	4981	C	ARG	B	405	58.326	56.448	27.502	1.00	7.63
ATOM	4982	O	ARG	B	405	59.227	55.625	27.338	1.00	8.53
ATOM	4983	N	PHE	B	406	57.138	56.338	26.919	1.00	4.12
ATOM	4984	CA	PHE	B	406	56.826	55.287	25.960	1.00	4.46
ATOM	4985	CB	PHE	B	406	55.369	55.413	25.536	1.00	6.67
ATOM	4986	CG	PHE	B	406	54.887	54.276	24.708	1.00	8.77
ATOM	4987	CD1	PHE	B	406	54.590	53.049	25.294	1.00	9.17
ATOM	4988	CE1	PHE	B	406	54.152	51.992	24.529	1.00	8.37
ATOM	4989	CZ	PHE	B	406	54.007	52.156	23.155	1.00	10.53
ATOM	4990	CE2	PHE	B	406	54.293	53.374	22.566	1.00	9.98
ATOM	4991	CD2	PHE	B	406	54.736	54.424	23.342	1.00	9.27
ATOM	4992	C	PHE	B	406	57.754	55.239	24.721	1.00	3.43
ATOM	4993	O	PHE	B	406	58.218	54.158	24.326	1.00	2.00
ATOM	4994	N	PHE	B	407	58.009	56.404	24.116	1.00	3.91
ATOM	4995	CA	PHE	B	407	59.014	56.549	23.042	1.00	5.09
ATOM	4996	CB	PHE	B	407	58.597	57.639	22.054	1.00	2.46
ATOM	4997	CG	PHE	B	407	57.241	57.449	21.470	1.00	2.00
ATOM	4998	CD1	PHE	B	407	56.246	58.389	21.700	1.00	2.00
ATOM	4999	CE1	PHE	B	407	54.978	58.231	21.160	1.00	2.00
ATOM	5000	CZ	PHE	B	407	54.704	57.125	20.363	1.00	2.00
ATOM	5001	CE2	PHE	B	407	55.695	56.176	20.119	1.00	2.00
ATOM	5002	CD2	PHE	B	407	56.961	56.350	20.669	1.00	2.00
ATOM	5003	C	PHE	B	407	60.444	56.845	23.566	1.00	5.86
ATOM	5004	O	PHE	B	407	61.052	57.870	23.233	1.00	3.30
ATOM	5005	N	ALA	B	408	60.973	55.927	24.371	1.00	7.79
ATOM	5006	CA	ALA	B	408	62.213	56.151	25.096	1.00	6.36
ATOM	5007	CB	ALA	B	408	62.287	55.232	26.301	1.00	2.74
ATOM	5008	C	ALA	B	408	63.442	55.980	24.201	1.00	10.98
ATOM	5009	O	ALA	B	408	64.261	56.907	24.059	1.00	13.54
ATOM	5010	N	GLY	B	409	63.579	54.803	23.597	1.00	12.32
ATOM	5011	CA	GLY	B	409	64.721	54.540	22.733	1.00	14.00
ATOM	5012	C	GLY	B	409	64.699	55.293	21.410	1.00	13.20
ATOM	5013	O	GLY	B	409	65.740	55.666	20.881	1.00	10.72
ATOM	5014	N	ILE	B	410	63.495	55.523	20.892	1.00	15.38
ATOM	5015	CA	ILE	B	410	63.283	56.052	19.546	1.00	12.78
ATOM	5016	CB	ILE	B	410	61.771	56.350	19.316	1.00	11.06
ATOM	5017	CG1	ILE	B	410	60.890	55.231	19.900	1.00	7.10
ATOM	5018	CD1	ILE	B	410	60.914	53.925	19.123	1.00	6.62
ATOM	5019	CG2	ILE	B	410	61.480	56.627	17.830	1.00	10.25
ATOM	5020	C	ILE	B	410	64.111	57.294	19.262	1.00	11.66
ATOM	5021	O	ILE	B	410	64.120	58.231	20.058	1.00	10.41

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	5022	N	VAL	B	411	64.818	57.275	18.136	1.00	11.48
ATOM	5023	CA	VAL	B	411	65.432	58.482	17.609	1.00	13.15
ATOM	5024	CB	VAL	B	411	66.853	58.254	17.122	1.00	14.89
ATOM	5025	CG1	VAL	B	411	67.651	59.547	17.257	1.00	15.43
ATOM	5026	CG2	VAL	B	411	67.508	57.106	17.890	1.00	15.87
ATOM	5027	C	VAL	B	411	64.560	59.009	16.472	1.00	14.19
ATOM	5028	O	VAL	B	411	64.385	58.353	15.440	1.00	12.26
ATOM	5029	N	TRP	B	412	64.021	60.208	16.679	1.00	15.19
ATOM	5030	CA	TRP	B	412	62.891	60.710	15.901	1.00	12.24
ATOM	5031	CB	TRP	B	412	62.198	61.846	16.649	1.00	8.88
ATOM	5032	CG	TRP	B	412	61.381	61.304	17.776	1.00	11.18
ATOM	5033	CD1	TRP	B	412	61.698	61.317	19.107	1.00	13.52
ATOM	5034	NE1	TRP	B	412	60.713	60.695	19.839	1.00	11.73
ATOM	5035	CE2	TRP	B	412	59.734	60.261	18.987	1.00	9.95
ATOM	5036	CD2	TRP	B	412	60.126	60.616	17.676	1.00	10.83
ATOM	5037	CE3	TRP	B	412	59.282	60.278	16.610	1.00	10.98
ATOM	5038	CZ3	TRP	B	412	58.108	59.610	16.879	1.00	12.18
ATOM	5039	CH2	TRP	B	412	57.752	59.266	18.196	1.00	11.83
ATOM	5040	CZ2	TRP	B	412	58.548	59.592	19.258	1.00	9.24
ATOM	5041	C	TRP	B	412	63.260	61.095	14.487	1.00	14.58
ATOM	5042	O	TRP	B	412	62.387	61.208	13.618	1.00	18.36
ATOM	5043	N	GLN	B	413	64.559	61.287	14.270	1.00	15.20
ATOM	5044	CA	GLN	B	413	65.117	61.552	12.953	1.00	14.61
ATOM	5045	CB	GLN	B	413	66.468	62.236	13.108	1.00	13.94
ATOM	5046	CG	GLN	B	413	66.982	62.876	11.849	1.00	15.29
ATOM	5047	CD	GLN	B	413	67.083	64.366	11.983	1.00	16.22
ATOM	5048	OE1	GLN	B	413	66.084	65.075	11.839	1.00	16.22
ATOM	5049	NE2	GLN	B	413	68.286	64.855	12.276	1.00	16.10
ATOM	5050	C	GLN	B	413	65.278	60.251	12.162	1.00	15.48
ATOM	5051	O	GLN	B	413	65.277	60.263	10.925	1.00	13.68
ATOM	5052	N	HIS	B	414	65.409	59.142	12.897	1.00	17.36
ATOM	5053	CA	HIS	B	414	65.685	57.816	12.337	1.00	17.09
ATOM	5054	CB	HIS	B	414	66.286	56.896	13.407	1.00	18.65
ATOM	5055	CG	HIS	B	414	67.776	56.791	13.357	1.00	19.06
ATOM	5056	ND1	HIS	B	414	68.550	57.516	12.477	1.00	19.59
ATOM	5057	CE1	HIS	B	414	69.822	57.217	12.664	1.00	21.56
ATOM	5058	NE2	HIS	B	414	69.901	56.325	13.635	1.00	21.97
ATOM	5059	CD2	HIS	B	414	68.635	56.043	14.087	1.00	19.80
ATOM	5060	C	HIS	B	414	64.411	57.185	11.831	1.00	16.07
ATOM	5061	O	HIS	B	414	64.361	56.673	10.708	1.00	13.91
ATOM	5062	N	VAL	B	415	63.387	57.218	12.686	1.00	17.18
ATOM	5063	CA	VAL	B	415	62.065	56.688	12.359	1.00	18.84
ATOM	5064	CB	VAL	B	415	61.112	56.666	13.615	1.00	16.46
ATOM	5065	CG1	VAL	B	415	60.902	58.053	14.205	1.00	15.76
ATOM	5066	CG2	VAL	B	415	59.785	56.014	13.292	1.00	16.70
ATOM	5067	C	VAL	B	415	61.511	57.475	11.162	1.00	19.55
ATOM	5068	O	VAL	B	415	60.721	56.961	10.372	1.00	20.16
ATOM	5069	N	TYR	B	416	61.983	58.711	11.034	1.00	18.88
ATOM	5070	CA	TYR	B	416	61.687	59.574	9.909	1.00	19.82
ATOM	5071	CB	TYR	B	416	62.009	61.017	10.301	1.00	19.35
ATOM	5072	CG	TYR	B	416	61.923	62.030	9.186	1.00	19.92
ATOM	5073	CD1	TYR	B	416	60.794	62.826	9.038	1.00	20.41

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	5074	CE1	TYR	B	416	60.709	63.763	8.027	1.00	22.09
ATOM	5075	CZ	TYR	B	416	61.769	63.921	7.152	1.00	21.94
ATOM	5076	OH	TYR	B	416	61.682	64.856	6.147	1.00	23.42
ATOM	5077	CE2	TYR	B	416	62.908	63.146	7.280	1.00	20.65
ATOM	5078	CD2	TYR	B	416	62.983	62.212	8.295	1.00	19.84
ATOM	5079	C	TYR	B	416	62.496	59.141	8.683	1.00	21.72
ATOM	5080	O	TYR	B	416	62.001	59.165	7.551	1.00	22.60
ATOM	5081	N	GLU	B	417	63.742	58.741	8.908	1.00	22.98
ATOM	5082	CA	GLU	B	417	64.603	58.311	7.811	1.00	22.62
ATOM	5083	CB	GLU	B	417	66.068	58.324	8.237	1.00	24.32
ATOM	5084	CG	GLU	B	417	66.875	59.467	7.647	1.00	27.05
ATOM	5085	CD	GLU	B	417	67.910	60.000	8.619	1.00	27.56
ATOM	5086	OE1	GLU	B	417	68.980	59.366	8.747	1.00	28.27
ATOM	5087	OE2	GLU	B	417	67.649	61.045	9.257	1.00	26.82
ATOM	5088	C	GLU	B	417	64.222	56.926	7.311	1.00	20.94
ATOM	5089	O	GLU	B	417	64.955	56.341	6.510	1.00	21.26
ATOM	5090	N	LYS	B	418	63.079	56.417	7.781	1.00	17.81
ATOM	5091	CA	LYS	B	418	62.594	55.080	7.437	1.00	17.59
ATOM	5092	CB	LYS	B	418	62.250	55.008	5.944	1.00	19.32
ATOM	5093	CG	LYS	B	418	60.805	54.677	5.610	1.00	20.49
ATOM	5094	CD	LYS	B	418	60.502	55.018	4.145	1.00	22.68
ATOM	5095	CE	LYS	B	418	60.147	53.778	3.326	1.00	23.26
ATOM	5096	NZ	LYS	B	418	58.767	53.874	2.753	1.00	24.01
ATOM	5097	C	LYS	B	418	63.622	54.002	7.818	1.00	18.01
ATOM	5098	O	LYS	B	418	63.679	52.932	7.206	1.00	16.37
ATOM	5099	N	LYS	B	419	64.433	54.299	8.833	1.00	20.05
ATOM	5100	CA	LYS	B	419	65.495	53.399	9.286	1.00	21.58
ATOM	5101	CB	LYS	B	419	66.681	54.203	9.836	1.00	21.79
ATOM	5102	CG	LYS	B	419	67.940	54.115	8.979	1.00	22.28
ATOM	5103	CD	LYS	B	419	68.717	55.425	8.986	1.00	22.60
ATOM	5104	CE	LYS	B	419	70.096	55.251	8.368	1.00	23.58
ATOM	5105	NZ	LYS	B	419	70.137	55.659	6.932	1.00	24.30
ATOM	5106	C	LYS	B	419	65.014	52.362	10.312	1.00	21.62
ATOM	5107	O	LYS	B	419	65.506	51.238	10.340	1.00	21.99
ATOM	5108	N	LEU	B	420	64.055	52.741	11.149	1.00	23.01
ATOM	5109	CA	LEU	B	420	63.474	51.825	12.127	1.00	25.14
ATOM	5110	CB	LEU	B	420	62.361	52.522	12.929	1.00	25.31
ATOM	5111	CG	LEU	B	420	62.550	52.506	14.454	1.00	24.73
ATOM	5112	CD1	LEU	B	420	63.098	53.835	14.988	1.00	22.15
ATOM	5113	CD2	LEU	B	420	61.264	52.114	15.173	1.00	24.48
ATOM	5114	C	LEU	B	420	62.934	50.588	11.422	1.00	25.34
ATOM	5115	O	LEU	B	420	62.066	50.696	10.557	1.00	25.10
ATOM	5116	N	SER	B	421	63.464	49.419	11.775	1.00	27.17
ATOM	5117	CA	SER	B	421	63.070	48.175	11.107	1.00	28.65
ATOM	5118	CB	SER	B	421	64.083	47.039	11.359	1.00	28.35
ATOM	5119	OG	SER	B	421	63.958	46.485	12.656	1.00	28.20
ATOM	5120	C	SER	B	421	61.645	47.780	11.499	1.00	27.57
ATOM	5121	O	SER	B	421	61.312	47.795	12.685	1.00	28.53
ATOM	5122	N	PRO	B	422	60.814	47.443	10.506	1.00	26.68
ATOM	5123	CA	PRO	B	422	59.390	47.170	10.731	1.00	26.88
ATOM	5124	CB	PRO	B	422	58.807	47.156	9.314	1.00	25.64
ATOM	5125	CG	PRO	B	422	59.912	46.735	8.466	1.00	26.93

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	5126	CD	PRO	B	422	61.174	47.271	9.089	1.00	27.56
ATOM	5127	C	PRO	B	422	59.181	45.822	11.398	1.00	26.38
ATOM	5128	O	PRO	B	422	60.054	44.966	11.277	1.00	27.83
ATOM	5129	N	PRO	B	423	58.069	45.640	12.104	1.00	26.23
ATOM	5130	CA	PRO	B	423	57.780	44.361	12.752	1.00	25.52
ATOM	5131	CB	PRO	B	423	56.851	44.761	13.907	1.00	27.42
ATOM	5132	CG	PRO	B	423	56.675	46.269	13.789	1.00	27.18
ATOM	5133	CD	PRO	B	423	57.012	46.630	12.377	1.00	27.44
ATOM	5134	C	PRO	B	423	57.080	43.378	11.815	1.00	23.99
ATOM	5135	O	PRO	B	423	56.980	42.200	12.164	1.00	22.27
ATOM	5136	N	PHE	B	424	56.624	43.847	10.652	1.00	23.26
ATOM	5137	CA	PHE	B	424	55.876	43.010	9.720	1.00	23.60
ATOM	5138	CB	PHE	B	424	54.377	43.165	9.975	1.00	23.98
ATOM	5139	CG	PHE	B	424	53.514	42.363	9.043	1.00	24.92
ATOM	5140	CD1	PHE	B	424	53.419	40.978	9.174	1.00	26.27
ATOM	5141	CE1	PHE	B	424	52.611	40.230	8.312	1.00	27.70
ATOM	5142	CZ	PHE	B	424	51.888	40.876	7.305	1.00	27.16
ATOM	5143	CE2	PHE	B	424	51.976	42.262	7.169	1.00	25.21
ATOM	5144	CD2	PHE	B	424	52.783	42.996	8.039	1.00	25.24
ATOM	5145	C	PHE	B	424	56.181	43.354	8.271	1.00	25.35
ATOM	5146	O	PHE	B	424	56.035	44.510	7.863	1.00	29.58
ATOM	5147	N	LYS	B	425	56.589	42.349	7.495	1.00	23.66
ATOM	5148	CA	LYS	B	425	56.860	42.520	6.066	1.00	21.08
ATOM	5149	CB	LYS	B	425	58.184	41.848	5.681	1.00	21.73
ATOM	5150	CG	LYS	B	425	59.366	42.803	5.539	1.00	23.54
ATOM	5151	CD	LYS	B	425	60.451	42.527	6.586	1.00	24.10
ATOM	5152	CE	LYS	B	425	61.829	42.962	6.093	1.00	23.74
ATOM	5153	NZ	LYS	B	425	62.735	41.797	5.865	1.00	21.37
ATOM	5154	C	LYS	B	425	55.715	41.945	5.230	1.00	19.06
ATOM	5155	O	LYS	B	425	55.531	40.731	5.199	1.00	18.70
ATOM	5156	N	PRO	B	426	54.930	42.813	4.585	1.00	18.34
ATOM	5157	CA	PRO	B	426	53.874	42.381	3.649	1.00	19.77
ATOM	5158	CB	PRO	B	426	53.444	43.697	2.986	1.00	17.71
ATOM	5159	CG	PRO	B	426	53.747	44.750	4.004	1.00	15.19
ATOM	5160	CD	PRO	B	426	54.961	44.281	4.742	1.00	15.73
ATOM	5161	C	PRO	B	426	54.331	41.341	2.593	1.00	22.96
ATOM	5162	O	PRO	B	426	55.115	41.654	1.691	1.00	23.51
ATOM	5163	N	GLN	B	427	53.821	40.113	2.714	1.00	26.14
ATOM	5164	CA	GLN	B	427	54.267	38.970	1.898	1.00	27.11
ATOM	5165	CB	GLN	B	427	54.142	37.662	2.701	1.00	28.14
ATOM	5166	CG	GLN	B	427	54.950	37.626	3.993	1.00	28.44
ATOM	5167	CD	GLN	B	427	56.389	37.204	3.769	1.00	28.57
ATOM	5168	OE1	GLN	B	427	56.768	36.090	4.122	1.00	29.24
ATOM	5169	NE2	GLN	B	427	57.193	38.089	3.181	1.00	28.25
ATOM	5170	C	GLN	B	427	53.508	38.837	0.575	1.00	26.04
ATOM	5171	O	GLN	B	427	52.528	38.093	0.481	1.00	26.48
ATOM	5172	N	VAL	B	428	53.976	39.535	-0.452	1.00	24.39
ATOM	5173	CA	VAL	B	428	53.219	39.633	-1.704	1.00	24.67
ATOM	5174	CB	VAL	B	428	53.196	41.090	-2.248	1.00	25.65
ATOM	5175	CG1	VAL	B	428	51.960	41.831	-1.738	1.00	23.03
ATOM	5176	CG2	VAL	B	428	54.493	41.843	-1.891	1.00	25.75
ATOM	5177	C	VAL	B	428	53.632	38.636	-2.810	1.00	22.99

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	5178	O	VAL	B	428	54.816	38.474	-3.108	1.00	19.93
ATOM	5179	N	THR	B	429	52.631	37.986	-3.406	1.00	23.47
ATOM	5180	CA	THR	B	429	52.818	37.047	-4.518	1.00	25.62
ATOM	5181	CB	THR	B	429	51.512	36.236	-4.793	1.00	26.66
ATOM	5182	OG1	THR	B	429	50.799	36.016	-3.571	1.00	27.48
ATOM	5183	CG2	THR	B	429	51.830	34.814	-5.282	1.00	27.23
ATOM	5184	C	THR	B	429	53.227	37.774	-5.799	1.00	25.59
ATOM	5185	O	THR	B	429	53.974	37.237	-6.628	1.00	25.49
ATOM	5186	N	SER	B	430	52.722	38.996	-5.947	1.00	23.73
ATOM	5187	CA	SER	B	430	52.862	39.774	-7.167	1.00	22.72
ATOM	5188	CB	SER	B	430	51.972	39.185	-8.267	1.00	22.21
ATOM	5189	OG	SER	B	430	50.801	38.583	-7.729	1.00	20.01
ATOM	5190	C	SER	B	430	52.427	41.195	-6.857	1.00	23.87
ATOM	5191	O	SER	B	430	51.927	41.461	-5.763	1.00	26.31
ATOM	5192	N	GLU	B	431	52.611	42.107	-7.809	1.00	24.94
ATOM	5193	CA	GLU	B	431	52.092	43.469	-7.673	1.00	26.95
ATOM	5194	CB	GLU	B	431	52.757	44.415	-8.681	1.00	27.82
ATOM	5195	CG	GLU	B	431	53.923	45.231	-8.130	1.00	29.51
ATOM	5196	CD	GLU	B	431	53.575	46.036	-6.881	1.00	32.06
ATOM	5197	OE1	GLU	B	431	52.469	46.622	-6.803	1.00	31.83
ATOM	5198	OE2	GLU	B	431	54.422	46.089	-5.963	1.00	34.08
ATOM	5199	C	GLU	B	431	50.554	43.513	-7.792	1.00	27.31
ATOM	5200	O	GLU	B	431	49.890	44.300	-7.102	1.00	25.43
ATOM	5201	N	THR	B	432	50.009	42.650	-8.655	1.00	27.75
ATOM	5202	CA	THR	B	432	48.560	42.483	-8.833	1.00	28.12
ATOM	5203	CB	THR	B	432	48.242	41.547	-10.043	1.00	26.38
ATOM	5204	OG1	THR	B	432	46.950	40.950	-9.879	1.00	24.96
ATOM	5205	CG2	THR	B	432	49.166	40.336	-10.079	1.00	25.65
ATOM	5206	C	THR	B	432	47.873	41.969	-7.564	1.00	31.24
ATOM	5207	O	THR	B	432	46.702	42.269	-7.321	1.00	32.54
ATOM	5208	N	ASP	B	433	48.617	41.204	-6.765	1.00	33.27
ATOM	5209	CA	ASP	B	433	48.101	40.545	-5.562	1.00	33.19
ATOM	5210	CB	ASP	B	433	49.185	39.648	-4.941	1.00	34.60
ATOM	5211	CG	ASP	B	433	48.750	39.003	-3.627	1.00	34.90
ATOM	5212	OD1	ASP	B	433	47.606	38.503	-3.533	1.00	34.60
ATOM	5213	OD2	ASP	B	433	49.503	38.942	-2.633	1.00	35.87
ATOM	5214	C	ASP	B	433	47.573	41.527	-4.525	1.00	31.69
ATOM	5215	O	ASP	B	433	48.231	42.527	-4.220	1.00	32.62
ATOM	5216	N	THR	B	434	46.377	41.224	-4.009	1.00	29.61
ATOM	5217	CA	THR	B	434	45.724	41.985	-2.938	1.00	26.44
ATOM	5218	CB	THR	B	434	44.499	42.765	-3.469	1.00	26.60
ATOM	5219	OG1	THR	B	434	43.625	41.870	-4.171	1.00	25.46
ATOM	5220	CG2	THR	B	434	44.910	43.789	-4.517	1.00	27.63
ATOM	5221	C	THR	B	434	45.268	41.052	-1.818	1.00	23.17
ATOM	5222	O	THR	B	434	44.095	41.046	-1.438	1.00	22.16
ATOM	5223	N	ARG	B	435	46.200	40.269	-1.288	1.00	19.68
ATOM	5224	CA	ARG	B	435	45.875	39.314	-0.240	1.00	16.54
ATOM	5225	CB	ARG	B	435	46.998	38.285	-0.068	1.00	15.91
ATOM	5226	CG	ARG	B	435	48.318	38.848	0.455	1.00	13.16
ATOM	5227	CD	ARG	B	435	49.323	37.785	0.902	1.00	11.43
ATOM	5228	NE	ARG	B	435	49.741	36.901	-0.190	1.00	7.98
ATOM	5229	CZ	ARG	B	435	49.522	35.590	-0.222	1.00	5.39

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	5230	NH1	ARG	B	435	48.889	34.988	0.776	1.00	5.35
ATOM	5231	NH2	ARG	B	435	49.934	34.876	-1.254	1.00	2.69
ATOM	5232	C	ARG	B	435	45.590	40.015	1.076	1.00	14.84
ATOM	5233	O	ARG	B	435	45.149	39.376	2.039	1.00	13.40
ATOM	5234	N	TYR	B	436	45.833	41.327	1.099	1.00	13.90
ATOM	5235	CA	TYR	B	436	45.738	42.123	2.326	1.00	14.53
ATOM	5236	CB	TYR	B	436	47.078	42.813	2.626	1.00	13.11
ATOM	5237	CG	TYR	B	436	48.158	41.852	3.066	1.00	12.11
ATOM	5238	CD1	TYR	B	436	49.367	41.769	2.378	1.00	12.28
ATOM	5239	CE1	TYR	B	436	50.370	40.877	2.775	1.00	14.02
ATOM	5240	CZ	TYR	B	436	50.160	40.045	3.872	1.00	16.17
ATOM	5241	OH	TYR	B	436	51.142	39.150	4.273	1.00	17.21
ATOM	5242	CE2	TYR	B	436	48.956	40.108	4.569	1.00	15.73
ATOM	5243	CD2	TYR	B	436	47.965	41.012	4.163	1.00	12.55
ATOM	5244	C	TYR	B	436	44.577	43.124	2.325	1.00	13.84
ATOM	5245	O	TYR	B	436	44.577	44.113	3.067	1.00	14.05
ATOM	5246	N	PHE	B	437	43.580	42.858	1.494	1.00	11.60
ATOM	5247	CA	PHE	B	437	42.395	43.696	1.466	1.00	10.70
ATOM	5248	CB	PHE	B	437	42.306	44.458	0.144	1.00	7.31
ATOM	5249	CG	PHE	B	437	43.381	45.490	-0.028	1.00	3.62
ATOM	5250	CD1	PHE	B	437	44.699	45.114	-0.267	1.00	3.17
ATOM	5251	CE1	PHE	B	437	45.692	46.060	-0.417	1.00	2.75
ATOM	5252	CZ	PHE	B	437	45.378	47.406	-0.333	1.00	2.75
ATOM	5253	CE2	PHE	B	437	44.071	47.795	-0.099	1.00	3.29
ATOM	5254	CD2	PHE	B	437	43.079	46.834	0.051	1.00	3.22
ATOM	5255	C	PHE	B	437	41.187	42.809	1.677	1.00	13.08
ATOM	5256	O	PHE	B	437	41.191	41.653	1.251	1.00	12.09
ATOM	5257	N	ASP	B	438	40.167	43.351	2.343	1.00	17.43
ATOM	5258	CA	ASP	B	438	38.947	42.611	2.681	1.00	21.30
ATOM	5259	CB	ASP	B	438	37.924	43.546	3.342	1.00	22.82
ATOM	5260	CG	ASP	B	438	37.892	43.411	4.868	1.00	25.30
ATOM	5261	OD1	ASP	B	438	37.062	42.623	5.374	1.00	24.74
ATOM	5262	OD2	ASP	B	438	38.641	44.059	5.642	1.00	27.09
ATOM	5263	C	ASP	B	438	38.337	41.890	1.462	1.00	23.31
ATOM	5264	O	ASP	B	438	38.342	42.420	0.341	1.00	25.71
ATOM	5265	N	GLU	B	439	37.828	40.678	1.688	1.00	22.87
ATOM	5266	CA	GLU	B	439	37.253	39.855	0.618	1.00	21.87
ATOM	5267	CB	GLU	B	439	37.118	38.395	1.073	1.00	25.82
ATOM	5268	CG	GLU	B	439	38.448	37.664	1.249	1.00	29.83
ATOM	5269	CD	GLU	B	439	38.590	36.446	0.344	1.00	31.99
ATOM	5270	OE1	GLU	B	439	38.059	35.368	0.710	1.00	33.40
ATOM	5271	OE2	GLU	B	439	39.236	36.561	-0.728	1.00	31.67
ATOM	5272	C	GLU	B	439	35.912	40.399	0.109	1.00	18.60
ATOM	5273	O	GLU	B	439	35.424	39.989	-0.942	1.00	17.16
ATOM	5274	N	GLU	B	440	35.335	41.329	0.864	1.00	16.37
ATOM	5275	CA	GLU	B	440	34.090	41.994	0.499	1.00	15.13
ATOM	5276	CB	GLU	B	440	33.507	42.691	1.729	1.00	17.49
ATOM	5277	CG	GLU	B	440	32.078	42.286	2.061	1.00	20.88
ATOM	5278	CD	GLU	B	440	31.132	43.472	2.151	1.00	22.30
ATOM	5279	OE1	GLU	B	440	30.007	43.297	2.681	1.00	23.27
ATOM	5280	OE2	GLU	B	440	31.511	44.576	1.690	1.00	21.80
ATOM	5281	C	GLU	B	440	34.287	43.009	-0.630	1.00	12.48

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	5282	O	GLU	B	440	33.327	43.430	-1.278	1.00	11.09
ATOM	5283	N	PHE	B	441	35.536	43.399	-0.853	1.00	10.88
ATOM	5284	CA	PHE	B	441	35.872	44.406	-1.844	1.00	12.26
ATOM	5285	CB	PHE	B	441	36.781	45.457	-1.226	1.00	11.29
ATOM	5286	CG	PHE	B	441	36.157	46.211	-0.106	1.00	11.12
ATOM	5287	CD1	PHE	B	441	36.829	46.357	1.102	1.00	9.74
ATOM	5288	CE1	PHE	B	441	36.261	47.067	2.148	1.00	9.36
ATOM	5289	CZ	PHE	B	441	35.002	47.637	1.996	1.00	9.86
ATOM	5290	CE2	PHE	B	441	34.317	47.500	0.792	1.00	11.80
ATOM	5291	CD2	PHE	B	441	34.898	46.793	-0.256	1.00	11.95
ATOM	5292	C	PHE	B	441	36.590	43.786	-3.024	1.00	15.98
ATOM	5293	O	PHE	B	441	36.371	44.176	-4.175	1.00	17.64
ATOM	5294	N	THR	B	442	37.458	42.822	-2.727	1.00	17.76
ATOM	5295	CA	THR	B	442	38.251	42.141	-3.749	1.00	18.76
ATOM	5296	CB	THR	B	442	39.442	41.384	-3.101	1.00	19.03
ATOM	5297	OG1	THR	B	442	39.062	40.872	-1.817	1.00	18.53
ATOM	5298	CG2	THR	B	442	40.564	42.360	-2.764	1.00	17.88
ATOM	5299	C	THR	B	442	37.433	41.225	-4.682	1.00	18.00
ATOM	5300	O	THR	B	442	37.894	40.892	-5.771	1.00	16.80
ATOM	5301	N	ALA	B	443	36.222	40.851	-4.262	1.00	18.77
ATOM	5302	CA	ALA	B	443	35.349	39.947	-5.022	1.00	21.39
ATOM	5303	CB	ALA	B	443	34.304	39.322	-4.103	1.00	19.73
ATOM	5304	C	ALA	B	443	34.676	40.549	-6.278	1.00	24.55
ATOM	5305	O	ALA	B	443	34.258	39.800	-7.172	1.00	24.41
ATOM	5306	N	GLN	B	444	34.572	41.882	-6.342	1.00	26.42
ATOM	5307	CA	GLN	B	444	34.003	42.582	-7.508	1.00	27.26
ATOM	5308	CB	GLN	B	444	33.185	43.801	-7.072	1.00	27.50
ATOM	5309	CG	GLN	B	444	31.918	43.477	-6.295	1.00	28.15
ATOM	5310	CD	GLN	B	444	31.930	44.059	-4.889	1.00	27.86
ATOM	5311	OE1	GLN	B	444	32.020	43.319	-3.910	1.00	28.20
ATOM	5312	NE2	GLN	B	444	31.835	45.383	-4.787	1.00	26.99
ATOM	5313	C	GLN	B	444	35.097	43.034	-8.476	1.00	27.45
ATOM	5314	O	GLN	B	444	36.141	43.536	-8.043	1.00	28.23
ATOM	5315	N	SER	B	445	34.850	42.868	-9.777	1.00	26.55
ATOM	5316	CA	SER	B	445	35.858	43.163	-10.806	1.00	26.44
ATOM	5317	CB	SER	B	445	36.364	41.865	-11.476	1.00	26.62
ATOM	5318	OG	SER	B	445	35.613	41.499	-12.627	1.00	25.91
ATOM	5319	C	SER	B	445	35.421	44.225	-11.837	1.00	26.45
ATOM	5320	O	SER	B	445	34.723	45.183	-11.484	1.00	24.53
ATOM	5321	N	ILE	B	446	35.845	44.032	-13.092	1.00	27.50
ATOM	5322	CA	ILE	B	446	35.634	44.967	-14.213	1.00	28.51
ATOM	5323	CB	ILE	B	446	35.826	44.252	-15.605	1.00	27.94
ATOM	5324	CG1	ILE	B	446	35.045	42.928	-15.678	1.00	27.10
ATOM	5325	CD1	ILE	B	446	34.396	42.649	-17.025	1.00	24.40
ATOM	5326	CG2	ILE	B	446	37.315	44.045	-15.921	1.00	27.20
ATOM	5327	C	ILE	B	446	34.302	45.730	-14.180	1.00	29.49
ATOM	5328	O	ILE	B	446	34.236	46.877	-13.724	1.00	29.43
TER	5328		ILE	B	446					
ATOM	5329	N	PRO	B	468	28.648	70.365	-13.352	1.00	31.71
ATOM	5330	CA	PRO	B	468	29.552	71.059	-12.428	1.00	32.09
ATOM	5331	CB	PRO	B	468	29.122	70.516	-11.064	1.00	31.84
ATOM	5332	CG	PRO	B	468	27.659	70.217	-11.231	1.00	31.61

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	5333	CD	PRO	B	468	27.470	69.805	-12.665	1.00	31.40
ATOM	5334	C	PRO	B	468	31.032	70.745	-12.700	1.00	32.65
ATOM	5335	O	PRO	B	468	31.418	69.576	-12.672	1.00	32.18
ATOM	5336	N	HIS	B	469	31.834	71.782	-12.961	1.00	33.78
ATOM	5337	CA	HIS	B	469	33.271	71.642	-13.246	1.00	34.47
ATOM	5338	CB	HIS	B	469	33.570	72.008	-14.718	1.00	31.97
ATOM	5339	CG	HIS	B	469	35.035	72.104	-15.052	1.00	29.73
ATOM	5340	ND1	HIS	B	469	35.813	71.000	-15.334	1.00	28.12
ATOM	5341	CE1	HIS	B	469	37.049	71.387	-15.598	1.00	26.57
ATOM	5342	NE2	HIS	B	469	37.101	72.703	-15.505	1.00	26.50
ATOM	5343	CD2	HIS	B	469	35.854	73.177	-15.171	1.00	28.51
ATOM	5344	C	HIS	B	469	34.124	72.493	-12.294	1.00	36.18
ATOM	5345	O	HIS	B	469	33.944	73.714	-12.216	1.00	37.23
ATOM	5346	N	PHE	B	470	35.043	71.842	-11.577	1.00	36.97
ATOM	5347	CA	PHE	B	470	36.012	72.541	-10.731	1.00	39.54
ATOM	5348	CB	PHE	B	470	36.027	71.976	-9.305	1.00	41.74
ATOM	5349	CG	PHE	B	470	34.868	72.423	-8.458	1.00	43.68
ATOM	5350	CD1	PHE	B	470	34.532	73.779	-8.356	1.00	44.66
ATOM	5351	CE1	PHE	B	470	33.449	74.195	-7.573	1.00	45.09
ATOM	5352	CZ	PHE	B	470	32.695	73.246	-6.882	1.00	45.24
ATOM	5353	CE2	PHE	B	470	33.026	71.887	-6.978	1.00	44.68
ATOM	5354	CD2	PHE	B	470	34.109	71.487	-7.759	1.00	43.87
ATOM	5355	C	PHE	B	470	37.413	72.467	-11.329	1.00	40.38
ATOM	5356	O	PHE	B	470	38.033	71.402	-11.325	1.00	40.25
ATOM	5357	N	PRO	B	471	37.913	73.593	-11.840	1.00	41.82
ATOM	5358	CA	PRO	B	471	39.256	73.635	-12.434	1.00	42.33
ATOM	5359	CB	PRO	B	471	39.234	74.926	-13.278	1.00	42.58
ATOM	5360	CG	PRO	B	471	37.822	75.471	-13.172	1.00	42.27
ATOM	5361	CD	PRO	B	471	37.249	74.908	-11.902	1.00	42.34
ATOM	5362	C	PRO	B	471	40.353	73.686	-11.360	1.00	41.63
ATOM	5363	O	PRO	B	471	40.039	73.631	-10.163	1.00	40.81
ATOM	5364	N	GLN	B	472	41.614	73.775	-11.795	1.00	40.44
ATOM	5365	CA	GLN	B	472	42.779	73.849	-10.901	1.00	38.23
ATOM	5366	CB	GLN	B	472	42.937	75.259	-10.317	1.00	38.18
ATOM	5367	CG	GLN	B	472	43.468	76.279	-11.318	1.00	37.65
ATOM	5368	CD	GLN	B	472	42.414	77.287	-11.739	1.00	37.19
ATOM	5369	OE1	GLN	B	472	41.639	77.036	-12.661	1.00	36.62
ATOM	5370	NE2	GLN	B	472	42.386	78.429	-11.067	1.00	37.32
ATOM	5371	C	GLN	B	472	42.727	72.780	-9.806	1.00	36.56
ATOM	5372	O	GLN	B	472	43.102	73.009	-8.652	1.00	35.16
ATOM	5373	N	PHE	B	473	42.241	71.612	-10.210	1.00	35.67
ATOM	5374	CA	PHE	B	473	42.162	70.427	-9.375	1.00	34.75
ATOM	5375	CB	PHE	B	473	40.706	69.924	-9.341	1.00	35.20
ATOM	5376	CG	PHE	B	473	40.540	68.501	-8.859	1.00	34.87
ATOM	5377	CD1	PHE	B	473	40.363	68.226	-7.509	1.00	34.27
ATOM	5378	CE1	PHE	B	473	40.197	66.916	-7.064	1.00	33.72
ATOM	5379	CZ	PHE	B	473	40.198	65.865	-7.974	1.00	33.78
ATOM	5380	CE2	PHE	B	473	40.363	66.126	-9.324	1.00	34.17
ATOM	5381	CD2	PHE	B	473	40.523	67.439	-9.764	1.00	34.81
ATOM	5382	C	PHE	B	473	43.125	69.393	-9.967	1.00	34.07
ATOM	5383	O	PHE	B	473	43.790	68.666	-9.231	1.00	35.52
ATOM	5384	N	ASP	B	474	43.209	69.357	-11.297	1.00	31.78

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	5385	CA	ASP	B	474	44.097	68.439	-12.005	1.00	30.92
ATOM	5386	CB	ASP	B	474	43.791	68.433	-13.501	1.00	32.01
ATOM	5387	CG	ASP	B	474	42.376	68.864	-13.803	1.00	33.67
ATOM	5388	OD1	ASP	B	474	41.548	67.991	-14.132	1.00	34.24
ATOM	5389	OD2	ASP	B	474	41.996	70.053	-13.725	1.00	34.34
ATOM	5390	C	ASP	B	474	45.563	68.784	-11.782	1.00	30.71
ATOM	5391	O	ASP	B	474	45.956	69.951	-11.846	1.00	29.55
ATOM	5392	N	TYR	B	475	46.357	67.749	-11.518	1.00	31.26
ATOM	5393	CA	TYR	B	475	47.787	67.879	-11.246	1.00	30.94
ATOM	5394	CB	TYR	B	475	48.010	68.210	-9.760	1.00	30.19
ATOM	5395	CG	TYR	B	475	49.106	67.394	-9.111	1.00	29.86
ATOM	5396	CD1	TYR	B	475	50.344	67.962	-8.827	1.00	29.95
ATOM	5397	CE1	TYR	B	475	51.360	67.210	-8.251	1.00	29.34
ATOM	5398	CZ	TYR	B	475	51.139	65.875	-7.963	1.00	28.52
ATOM	5399	OH	TYR	B	475	52.136	65.127	-7.392	1.00	29.27
ATOM	5400	CE2	TYR	B	475	49.922	65.285	-8.243	1.00	28.61
ATOM	5401	CD2	TYR	B	475	48.913	66.042	-8.808	1.00	29.15
ATOM	5402	C	TYR	B	475	48.549	66.595	-11.637	1.00	31.37
ATOM	5403	O	TYR	B	475	47.954	65.511	-11.717	1.00	30.37
ATOM	5404	N	SER	B	476	49.859	66.730	-11.874	1.00	31.87
ATOM	5405	CA	SER	B	476	50.764	65.582	-12.042	1.00	31.69
ATOM	5406	CB	SER	B	476	50.757	65.089	-13.491	1.00	31.24
ATOM	5407	OG	SER	B	476	49.672	64.202	-13.700	1.00	31.01
ATOM	5408	C	SER	B	476	52.200	65.865	-11.563	1.00	31.81
ATOM	5409	O	SER	B	476	52.584	67.026	-11.379	1.00	31.72
ATOM	5410	N	ALA	B	477	52.981	64.799	-11.364	1.00	31.55
ATOM	5411	CA	ALA	B	477	54.346	64.902	-10.833	1.00	32.22
ATOM	5412	CB	ALA	B	477	54.406	64.316	-9.422	1.00	32.63
ATOM	5413	C	ALA	B	477	55.408	64.248	-11.728	1.00	32.51
ATOM	5414	O	ALA	B	477	55.221	64.122	-12.939	1.00	33.28
ATOM	5415	N	SER	B	478	56.526	63.850	-11.120	1.00	32.63
ATOM	5416	CA	SER	B	478	57.600	63.153	-11.821	1.00	32.96
ATOM	5417	CB	SER	B	478	58.605	64.154	-12.393	1.00	32.47
ATOM	5418	OG	SER	B	478	59.359	63.564	-13.437	1.00	32.85
ATOM	5419	C	SER	B	478	58.305	62.158	-10.898	1.00	33.82
ATOM	5420	O	SER	B	478	59.219	61.441	-11.313	1.00	34.50
TER Peptide B										
ATOM	5421	N	GLY	B	3	36.231	42.092	16.828	1.00	77.87
ATOM	5422	CA	GLY	B	3	35.401	42.391	15.627	1.00	77.15
ATOM	5423	C	GLY	B	3	35.352	43.871	15.292	1.00	74.66
ATOM	5424	O	GLY	B	3	36.306	44.419	14.743	1.00	76.35
ATOM	5425	N	ARG	B	4	34.229	44.501	15.626	1.00	71.60
ATOM	5426	CA	ARG	B	4	33.958	45.920	15.361	1.00	70.81
ATOM	5427	CB	ARG	B	4	34.880	46.840	16.177	1.00	68.89
ATOM	5428	CG	ARG	B	4	35.299	48.145	15.535	1.00	67.82
ATOM	5429	CD	ARG	B	4	36.807	48.232	15.413	1.00	69.37
ATOM	5430	NE	ARG	B	4	37.335	49.547	15.065	1.00	69.01
ATOM	5431	CZ	ARG	B	4	37.226	50.115	13.867	1.00	69.46
ATOM	5432	NH1	ARG	B	4	36.573	49.505	12.884	1.00	66.67
ATOM	5433	NH2	ARG	B	4	37.766	51.308	13.653	1.00	70.36
ATOM	5434	C	ARG	B	4	33.901	46.257	13.863	1.00	73.54
ATOM	5435	O	ARG	B	4	34.876	46.061	13.126	1.00	73.45

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	5436	N	PRO	B	5	32.740	46.754	13.426	1.00	74.33
ATOM	5437	CA	PRO	B	5	32.453	46.937	11.999	1.00	73.21
ATOM	5438	CB	PRO	B	5	30.985	47.379	12.001	1.00	74.87
ATOM	5439	CG	PRO	B	5	30.791	48.025	13.333	1.00	74.29
ATOM	5440	CD	PRO	B	5	31.614	47.200	14.269	1.00	73.53
ATOM	5441	C	PRO	B	5	33.313	48.032	11.405	1.00	71.42
ATOM	5442	O	PRO	B	5	33.799	48.865	12.168	1.00	72.08
ATOM	5443	N	ARG	B	6	33.497	48.023	10.084	1.00	70.45
ATOM	5444	CA	ARG	B	6	34.164	49.122	9.392	1.00	69.90
ATOM	5445	CB	ARG	B	6	34.160	48.902	7.877	1.00	71.75
ATOM	5446	CG	ARG	B	6	35.329	48.069	7.363	1.00	75.17
ATOM	5447	CD	ARG	B	6	35.588	48.186	5.858	1.00	78.38
ATOM	5448	NE	ARG	B	6	36.777	48.986	5.521	1.00	81.20
ATOM	5449	CZ	ARG	B	6	36.758	50.271	5.128	1.00	82.44
ATOM	5450	NH1	ARG	B	6	35.614	50.944	5.029	1.00	82.43
ATOM	5451	NH2	ARG	B	6	37.894	50.893	4.837	1.00	81.60
ATOM	5452	C	ARG	B	6	33.468	50.430	9.763	1.00	68.05
ATOM	5453	O	ARG	B	6	32.248	50.528	9.718	1.00	64.87
ATOM	5454	N	THR	B	7	34.249	51.418	10.177	1.00	69.96
ATOM	5455	CA	THR	B	7	33.681	52.676	10.641	1.00	75.31
ATOM	5456	CB	THR	B	7	34.371	53.180	11.937	1.00	78.86
ATOM	5457	OG1	THR	B	7	35.759	53.446	11.691	1.00	81.18
ATOM	5458	CG2	THR	B	7	34.386	52.102	13.023	1.00	79.41
ATOM	5459	C	THR	B	7	33.772	53.725	9.547	1.00	75.83
ATOM	5460	O	THR	B	7	34.782	53.815	8.849	1.00	77.51
ATOM	5461	N	THR	B	8	32.713	54.516	9.411	1.00	75.65
ATOM	5462	CA	THR	B	8	32.593	55.466	8.314	1.00	75.25
ATOM	5463	CB	THR	B	8	31.315	55.177	7.534	1.00	77.85
ATOM	5464	OG1	THR	B	8	31.376	53.832	7.041	1.00	81.44
ATOM	5465	CG2	THR	B	8	31.237	56.020	6.256	1.00	80.03
ATOM	5466	C	THR	B	8	32.619	56.905	8.801	1.00	73.48
ATOM	5467	O	THR	B	8	32.054	57.236	9.839	1.00	76.37
ATOM	5468	N	SER	B	9	33.287	57.757	8.041	1.00	69.64
ATOM	5469	CA	SER	B	9	33.400	59.154	8.400	1.00	68.59
ATOM	5470	CB	SER	B	9	34.571	59.780	7.659	1.00	71.13
ATOM	5471	OG	SER	B	9	34.367	59.686	6.265	1.00	71.72
ATOM	5472	C	SER	B	9	32.120	59.912	8.077	1.00	66.52
ATOM	5473	O	SER	B	9	31.226	59.391	7.417	1.00	66.44
ATOM	5474	N	PHE	B	10	32.045	61.146	8.556	1.00	63.50
ATOM	5475	CA	PHE	B	10	30.918	62.013	8.293	1.00	64.59
ATOM	5476	CB	PHE	B	10	29.815	61.795	9.333	1.00	62.46
ATOM	5477	CG	PHE	B	10	30.143	62.359	10.674	1.00	61.36
ATOM	5478	CD1	PHE	B	10	29.911	63.697	10.956	1.00	60.08
ATOM	5479	CE1	PHE	B	10	30.240	64.235	12.202	1.00	62.01
ATOM	5480	CZ	PHE	B	10	30.800	63.428	13.183	1.00	62.27
ATOM	5481	CE2	PHE	B	10	31.038	62.083	12.914	1.00	62.88
ATOM	5482	CD2	PHE	B	10	30.713	61.557	11.658	1.00	63.57
ATOM	5483	C	PHE	B	10	31.402	63.448	8.369	1.00	69.31
ATOM	5484	O	PHE	B	10	32.478	63.719	8.915	1.00	71.93
ATOM	5485	N	ALA	B	11	30.596	64.356	7.819	1.00	72.01
ATOM	5486	CA	ALA	B	11	30.762	65.791	8.000	1.00	71.64
ATOM	5487	CB	ALA	B	11	31.710	66.335	6.964	1.00	71.14

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	5488	C	ALA	B	11	29.387	66.454	7.888	1.00	74.07
ATOM	5489	O	ALA	B	11	28.549	66.015	7.085	1.00	73.91
ATOM	5490	N	GLU	B	12	29.138	67.466	8.723	1.00	75.99
ATOM	5491	CA	GLU	B	12	27.940	68.308	8.598	1.00	81.61
ATOM	5492	CB	GLU	B	12	26.760	67.837	9.473	1.00	85.80
ATOM	5493	CG	GLU	B	12	26.862	66.434	10.062	1.00	93.38
ATOM	5494	CD	GLU	B	12	25.640	65.554	9.792	1.00	97.62
ATOM	5495	OE1	GLU	B	12	25.403	65.186	8.608	1.00	97.70
ATOM	5496	OE2	GLU	B	12	24.932	65.206	10.774	1.00	98.65
ATOM	5497	C	GLU	B	12	28.273	69.764	8.909	1.00	82.88
ATOM	5498	O	GLU	B	12	28.527	70.150	10.057	1.00	82.74
ATOM	5499	OXT	GLU	B	12	28.297	70.587	7.996	1.00	84.03
TER										
ATOM	5500	O1A	ANP	B	490	40.736	56.269	0.517	1.00	65.98
ATOM	5501	PA	ANP	B	490	39.476	56.089	1.472	1.00	61.95
ATOM	5502	O2A	ANP	B	490	39.897	56.090	3.006	1.00	66.24
ATOM	5503	O3A	ANP	B	490	38.388	57.226	1.183	1.00	61.27
ATOM	5504	PB	ANP	B	490	37.100	57.408	2.117	1.00	62.59
ATOM	5505	O1B	ANP	B	490	35.992	56.356	1.692	1.00	63.01
ATOM	5506	O2B	ANP	B	490	36.529	58.891	1.975	1.00	63.56
ATOM	5507	N3B	ANP	B	490	37.450	57.086	3.790	1.00	64.14
ATOM	5508	PG	ANP	B	490	36.137	57.418	4.889	1.00	64.32
ATOM	5509	O3G	ANP	B	490	34.807	56.669	4.445	1.00	65.34
ATOM	5510	O2G	ANP	B	490	36.496	56.934	6.358	1.00	65.52
ATOM	5511	O1G	ANP	B	490	35.951	58.991	4.823	1.00	65.40
ATOM	5512	O5*	ANP	B	490	38.751	54.712	1.172	1.00	61.60
ATOM	5513	C5*	ANP	B	490	38.712	53.784	2.243	1.00	61.27
ATOM	5514	C4*	ANP	B	490	39.627	52.630	1.896	1.00	58.60
ATOM	5515	O4*	ANP	B	490	40.314	52.868	0.674	1.00	54.17
ATOM	5516	C1*	ANP	B	490	41.505	52.094	0.707	1.00	59.26
ATOM	5517	C2*	ANP	B	490	41.778	51.721	2.162	1.00	59.70
ATOM	5518	O2*	ANP	B	490	41.700	50.315	2.367	1.00	59.84
ATOM	5519	C3*	ANP	B	490	40.693	52.410	2.947	1.00	59.23
ATOM	5520	O3*	ANP	B	490	40.222	51.570	3.987	1.00	60.77
ATOM	5521	N9	ANP	B	490	42.621	52.930	0.219	1.00	60.78
ATOM	5522	C8	ANP	B	490	42.693	54.283	0.151	1.00	60.89
ATOM	5523	N7	ANP	B	490	43.885	54.735	-0.350	1.00	59.27
ATOM	5524	C5	ANP	B	490	44.614	53.641	-0.610	1.00	59.75
ATOM	5525	C6	ANP	B	490	45.948	53.278	-1.145	1.00	61.98
ATOM	5526	N6	ANP	B	490	46.816	54.237	-1.535	1.00	63.69
ATOM	5527	C4	ANP	B	490	43.781	52.513	-0.231	1.00	60.40
ATOM	5528	N3	ANP	B	490	44.220	51.151	-0.368	1.00	62.24
ATOM	5529	C2	ANP	B	490	45.459	50.958	-0.871	1.00	66.35
ATOM	5530	N1	ANP	B	490	46.289	51.968	-1.239	1.00	64.75
ATOM	5531	MN	MN	B	491	38.911	56.563	5.142	1.00	59.48
ATOM	5532	MN	MN	B	492	37.513	60.211	4.000	1.00	70.66
TER										
ATOM	5533	O	HOH	B	500	56.696	41.781	18.932	1.00	33.51
ATOM	5534	O	HOH	B	501	35.997	61.332	33.177	1.00	37.49
ATOM	5535	O	HOH	B	502	39.275	47.725	17.172	1.00	24.72
ATOM	5536	O	HOH	B	503	36.156	54.959	20.848	1.00	26.79
ATOM	5537	O	HOH	B	504	33.232	51.144	26.038	1.00	26.58

FIGURE 3 (Cont.)

	A	B	C	D	E	F	G	H	I	J
ATOM	5538	O	HOH	B	505	35.734	56.074	38.054	1.00	41.80
ATOM	5539	O	HOH	B	506	50.924	58.731	34.338	1.00	7.07
ATOM	5540	O	HOH	B	507	40.791	64.735	30.804	1.00	47.25
ATOM	5541	O	HOH	B	508	-0.883	-4.548	23.859	1.00	31.17
ATOM	5542	O	HOH	B	509	9.604	-5.253	44.274	1.00	31.40
ATOM	5543	O	HOH	B	510	8.342	-14.502	50.113	1.00	48.29
ATOM	5544	O	HOH	B	511	0.427	-11.693	32.465	1.00	40.80
ATOM	5545	O	HOH	B	512	-5.380	-4.103	45.084	1.00	41.45
ATOM	5546	O	HOH	B	513	-12.592	16.204	51.921	1.00	30.04
ATOM	5547	O	HOH	B	514	-12.237	10.744	55.180	1.00	28.58
ATOM	5548	O	HOH	B	515	57.986	48.033	27.056	1.00	42.67
ATOM	5549	O	HOH	B	516	56.656	47.677	30.807	1.00	33.50
ATOM	5550	O	HOH	B	517	31.789	70.556	16.103	1.00	42.31
ATOM	5551	O	HOH	B	518	29.791	54.625	12.185	1.00	50.25

FIGURE 4A

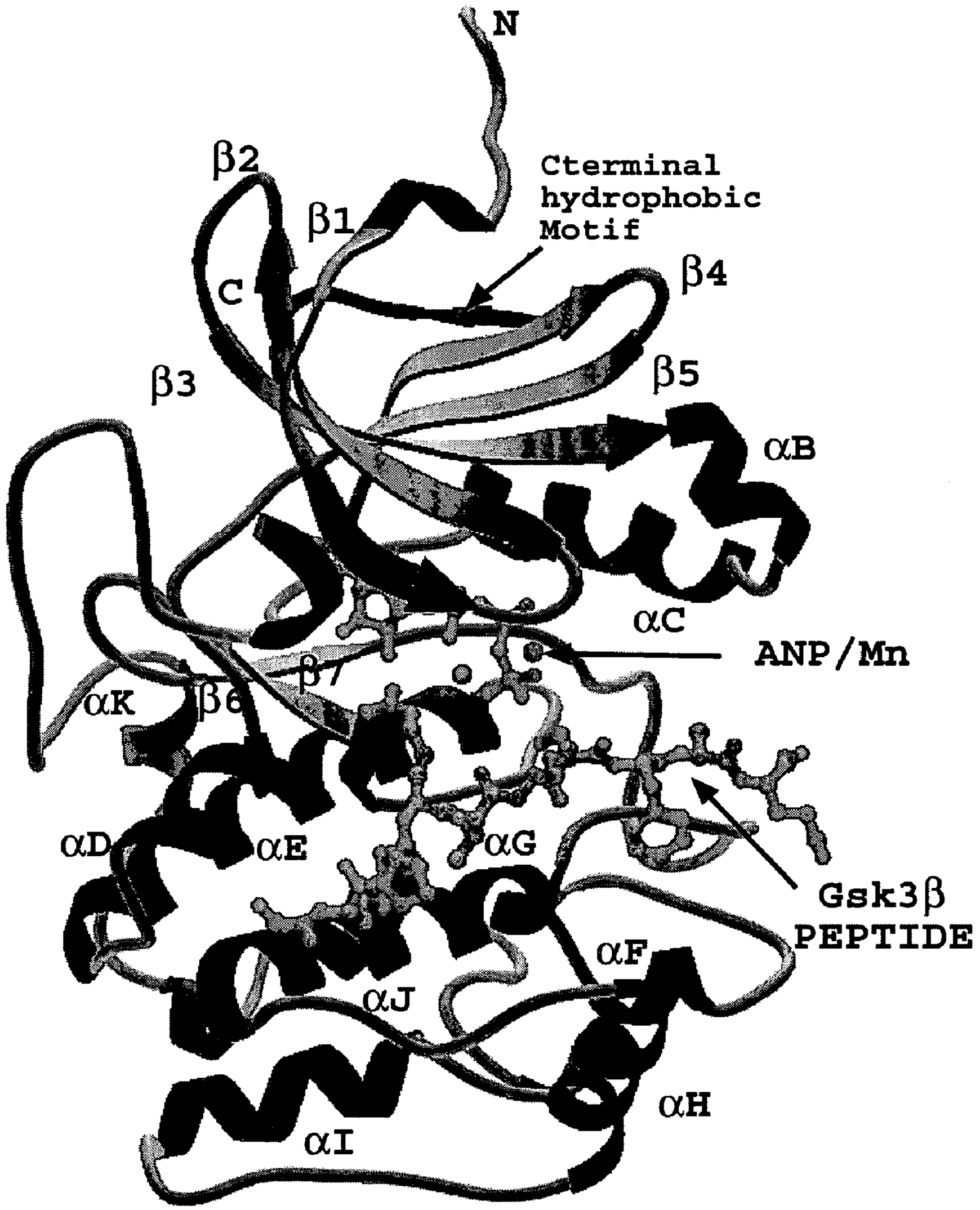

N
β2
β1
Cterminal
hydrophobic
Motif
C
β4
β3
β5
αB
αC
ANP/Mn
β7
αK
β6
αD
αE
αG
Gsk3β
PEPTIDE
αF
αJ
αH
αI

FIGURE 4B

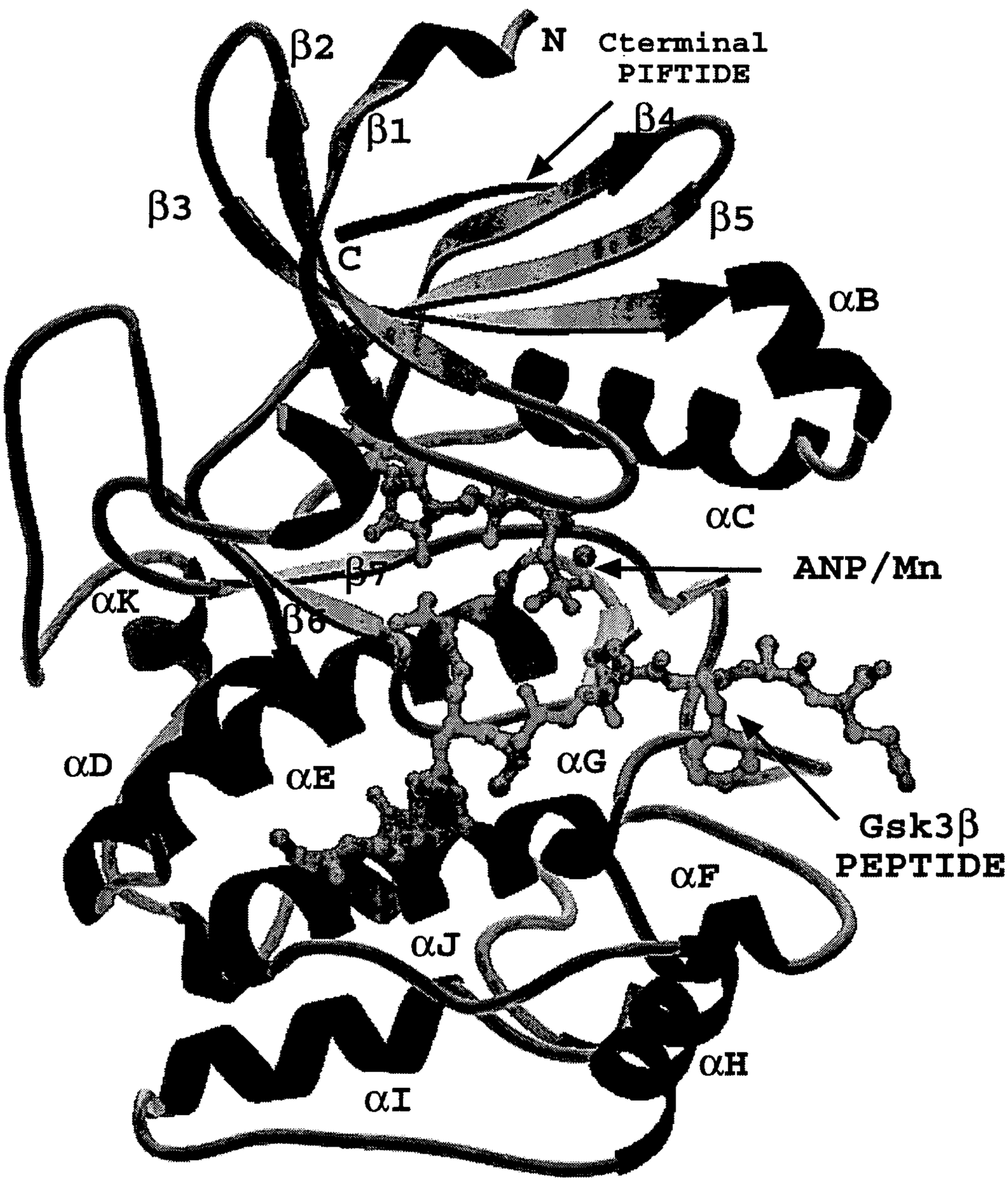

β2
N
Cterminal
PIFTIDE
β1
β4
β3
β5
C
αB
αC
β7
ANP/Mn
αK
β6
αD
αE
αG
Gsk3β
PEPTIDE
αF
αJ
αH
αI

FIGURE 5

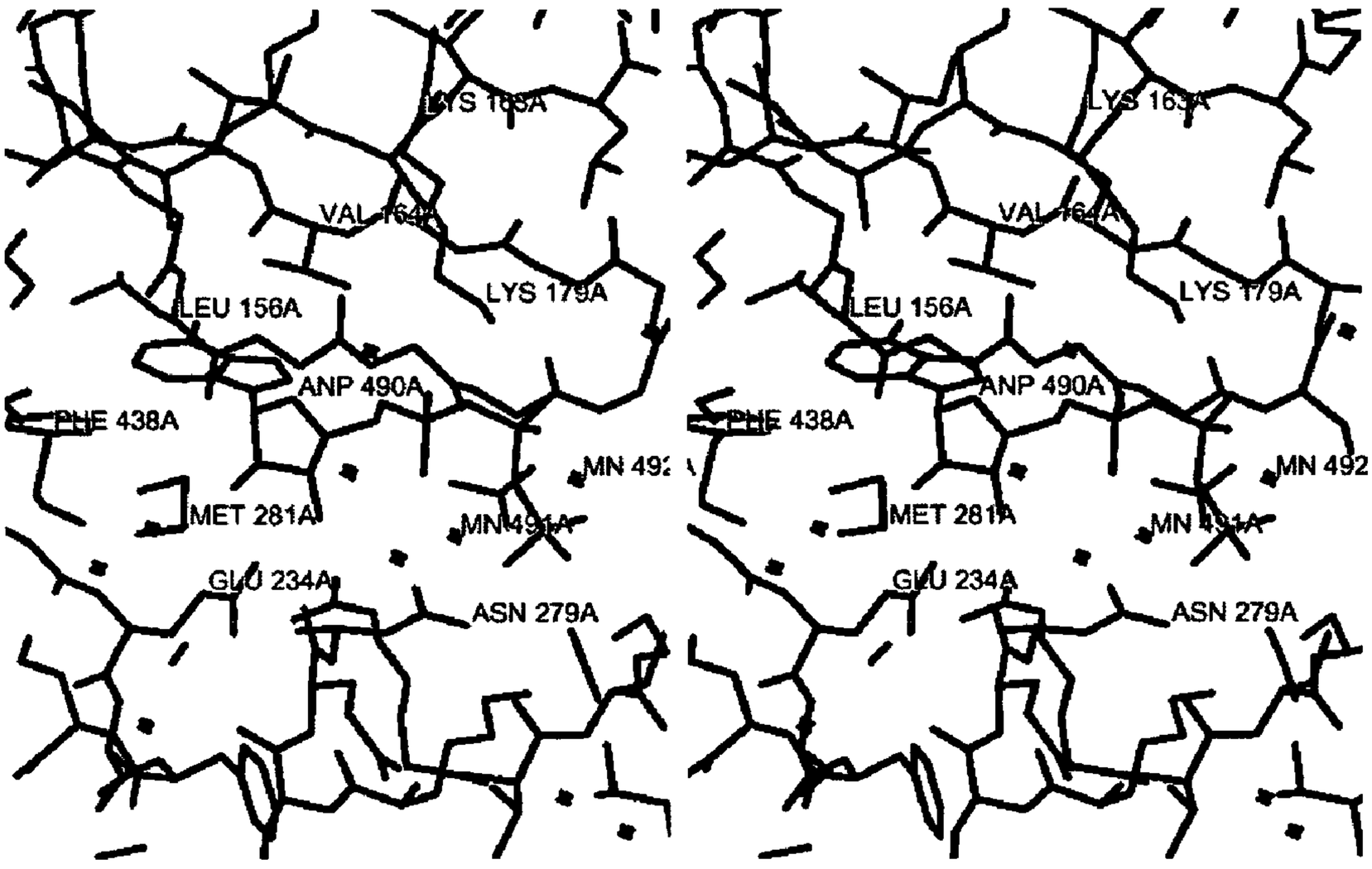
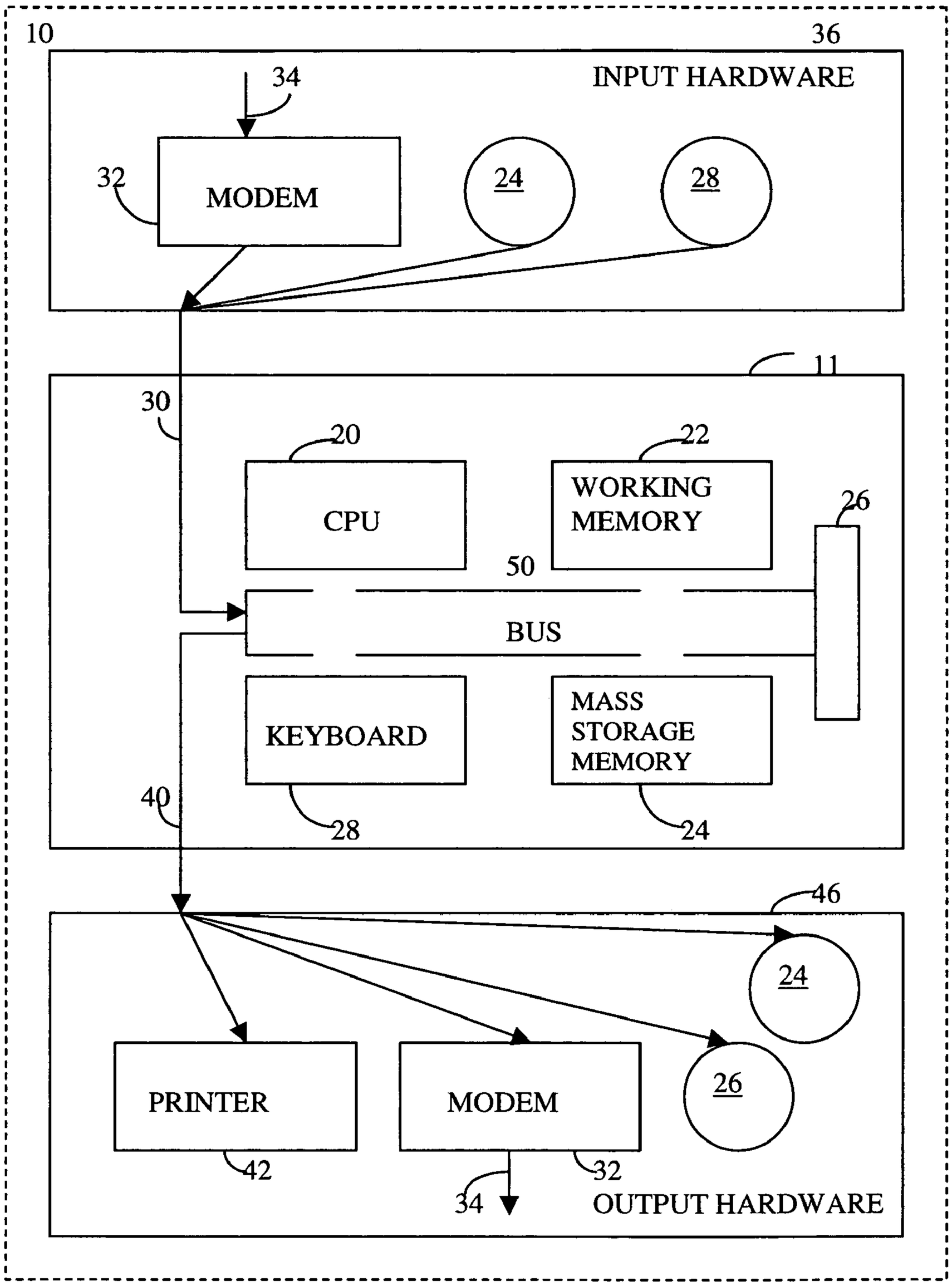

LYS 163A
VAL 164A
LEU 156A
LYS 179A
ANP 490A
PHE 438A
MN 492
MET 281A
MN 491A
GLU 234A
ASN 279A
LYS 163A
VAL 164A
LEU 156A
LYS 179A
ANP 490A
PHE 438A
MN 492
MET 281A
MN 491A
GLU 234A
ASN 279A

FIGURE 6


10
36
INPUT HARDWARE
34
32
MODEM
24
28
11
30
20
CPU
22
WORKING MEMORY
26
50
BUS
KEYBOARD
MASS STORAGE MEMORY
40
28
24
46
24
PRINTER
MODEM
26
42
32
34
OUTPUT HARDWARE

CRYSTALLIZATION OF PROTEIN KINASE Bα/AKT1

FIELD OF THE INVENTION

The present invention relates to a member of a family of Serine/Threonine protein kinases and more specifically to a particular protein kinase known as Protein Kinase Bα/AKT1 (AKT1). Provided are AKT1 in crystalline form, methods of forming crystals comprising AKT1, methods of using crystals comprising AKT1, a crystal structure of AKT1, and methods of using the crystal structure.

BACKGROUND OF THE INVENTION

A general approach to designing inhibitors that are selective for a given protein is to determine how a putative inhibitor interacts with a three dimensional structure of that protein. For this reason it is useful to obtain the protein in crystalline form and perform X-ray diffraction techniques to determine the protein's three-dimensional structure coordinates. Various methods for preparing crystalline proteins are known in the art.

Once protein crystals are produced, crystallographic data can be generated using the crystals to provide useful structural information that assists in the design of small molecules that bind to the active site of the protein and inhibit the protein's activity in vivo. If the protein is crystallized as a complex with a ligand, one can determine both the shape of the protein's binding pocket when bound to the ligand, as well as the amino acid residues that are capable of close contact with the ligand. By knowing the shape and amino acid residues comprised in the binding pocket, one may design new ligands that will interact favorably with the protein. With such structural information, available computational methods may be used to predict how strong the ligand binding interaction will be. Such methods aid in the design of inhibitors that bind strongly, as well as selectively to the protein. A need thus exists for proteins in crystalline form.

SUMMARY OF THE INVENTION

The present invention is directed to crystals comprising AKT1 and particularly crystals comprising AKT1 that have sufficient size and quality to obtain useful information about the structural properties of AKT1 and molecules or complexes that may associate with AKT1.

In one embodiment, a composition is provided that comprises a protein in crystalline form wherein at least a portion of the protein has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with residues 29 to 370 of SEQ. ID No. 3.

In another embodiment, a composition is provided that comprises a protein in crystalline form wherein at least a portion of the protein has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with residues 29 to 350 of SEQ. ID No. 5.

In one variation, the protein has activity characteristic of AKT1. For example, the protein may optionally be inhibited by inhibitors of wild type AKT1. The protein crystal may also diffract X-rays for a determination of structure coordinates to a resolution of 4 Å, 3.5 Å, 3.0 Å or less.

In one variation, the protein crystal has a crystal lattice in a C2 space group. The protein crystal may also have a crystal lattice having unit cell dimensions, +/−5%, of a=153.000 Å, b=79.597 Å, c=103.363 Å, α=90.00, β=123.16, γ=90.00 degrees.

In another variation, the protein crystal has a crystal lattice in a P1 space group. The protein crystal may also have a crystal lattice having unit cell dimensions, +/−5%, of a=44.045 Å, b=45.247 Å, c=101.445 Å, α=88.41, β=78.93, γ=72.99 degrees.

The present invention is also directed to crystallizing AKT1. The present invention is also directed to the conditions useful for crystallizing AKT1. It should be recognized that a wide variety of crystallization methods can be used in combination with the crystallization conditions to form crystals comprising AKT1 including, but not limited to, vapor diffusion, batch, dialysis, and other methods of contacting the protein solution for the purpose of crystallization.

In one embodiment, a method is provided for forming crystals of a protein comprising: forming a crystallization volume comprising: a protein wherein at least a portion of the protein has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with residues 29 to 370 of SEQ. ID No. 3; and storing the crystallization volume under conditions suitable for crystal formation.

In another embodiment, a method is provided for forming crystals of a protein comprising: forming a crystallization volume comprising: a protein wherein at least a portion of the protein has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with residues 29 to 350 of SEQ. ID No. 5; and storing the crystallization volume under conditions suitable for crystal formation.

In one variation, the crystallization volume comprises the protein, a two-fold molar excess of a GSK3β substrate peptide (SEQ ID NO:6), a nucleotide or nucleotide analog such as adenosine-5'-[(β,γ)-imido]triphosphate (AMPPNP), a two-fold molar excess of $MnCl_2$, and crystallization solutions comprising 19% polyethylene glycol 3350, 0.20M potassium chloride and 0.1 M N-[2-Hydroxyethyl]piperazine-N'-[2-ethanesulfonic acid](HEPES), pH7.5.

The method may optionally further comprise forming a protein crystal that has a crystal lattice in a C2 space group. The method also optionally further comprises forming a protein crystal that has a crystal lattice having unit cell dimensions, +/−5%, of a=153.000 Å, b=79.597 Å, c=103.363 Å, α=90.00, β=123.16, γ=90.00 degrees. The invention also relates to protein crystals formed by these methods.

In another variation, the crystallization volume comprises the protein, a two-fold molar excess of a GSK3β substrate peptide (GRPRTTSFAE) (SEQ ID NO:6), a nucleotide or nucleotide analog such as adenosine-5'-[(β,γ-imido]triphosphate (AMPPNP), a two-fold molar excess of $MnCl_2$, and crystallization solutions comprising 13% polyethylene glycol 3350, 0.20M ammonium sulfate and 0.1M N-[2-Hydroxyethyl]piperazine-N'-[2-ethanesulfonic acid](HEPES), pH 7.5.

The method may optionally further comprise forming a protein crystal that has a crystal lattice in a P1 space group. The method also optionally further comprises forming a protein crystal that has a crystal lattice having unit cell dimensions, +/−5%, of a=44.045 Å, b=45.247 Å, c=101.445 Å, α=88.41, β=78.93, γ=72.99 degrees. The invention also relates to protein crystals formed by these methods.

The present invention is also directed to a composition comprising an isolated protein that comprises or consists of one or more of the protein sequence(s) of AKT1 taught herein for crystallizing AKT1. The present invention is also directed to a composition comprising an isolated nucleic acid molecule that comprises or consists of the nucleotides for expressing the protein sequence of AKT1 taught herein for crystallizing AKT1.

The present invention is also directed to an expression vector that may be used to express the isolated proteins taught herein for crystallizing AKT1. In one variation, the expression vector comprises a promoter that promotes expression of the isolated protein.

The present invention is also directed to a cell line transformed or transfected by an isolated nucleic acid molecule or expression vector of the present invention.

The present invention is also directed to structure coordinates for AKT1 as well as structure coordinates that are comparatively similar to these structure coordinates. It is noted that these comparatively similar structure coordinates may encompass proteins with similar sequences and/or structures, such as other protein kinases. For example, machine-readable data storage media is provided having data storage material encoded with machine-readable data that comprises structure coordinates that are comparatively similar to the structure coordinates of AKT1. The present invention is also directed to a machine readable data storage medium having data storage material encoded with machine readable data, which, when read by an appropriate machine, can display a three dimensional representation of all or a portion of a structure of AKT1 or a model that is comparatively similar to the structure of all or a portion of AKT1.

Various embodiments of machine readable data storage medium are provided that comprise data storage material encoded with machine readable data. The machine readable data comprises: structure coordinates that have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1. The amino acids being overlayed and compared need not be identical when the RMSD calculation is performed on alpha carbons and main chain atoms but the amino acids being overlayed and compared must have identical side chains when the RMSD calculation is performed on all non-hydrogen atoms.

For example, in one embodiment where the comparison is based on the 4 Angstrom set of amino acid residues (Column 1) and is based on superimposing alpha-carbon atoms (Column 2), the structure coordinates may have a root mean square deviation equal to or less than 0.22 when compared to the structure coordinates of FIG. **3**.

TABLE 1

AA RESIDUES TO USE TO PERFORM RMSD COMPARISON	PORTION OF EACH AA RESIDUE USED TO PERFORM RMSD COMPARISON	RMSD VALUE LESS THAN OR EQUAL TO		
Table 2 (4 Angstrom set)	alpha-carbon atoms[1]	0.22	0.14	0.11
	main-chain atoms[1]	0.25	0.16	0.12
	all non-hydrogen[2]	0.27	0.18	0.13
Table 3 (7 Angstrom set)	alpha-carbon atoms[1]	0.25	0.17	0.13
	main-chain atoms[1]	0.29	0.19	0.14
	all non-hydrogen[2]	0.34	0.22	0.17
Table 4 (10 Angstrom set)	alpha-carbon atoms[1]	0.30	0.20	0.15
	main-chain atoms[1]	0.31	0.21	0.16
	all non-hydrogen[2]	0.40	0.26	0.20
Residues 138 to 480 of SEQ. ID No. 1	alpha-carbon atoms[1]	0.40	0.26	0.21
	main-chain atoms[1]	0.40	0.27	0.20
	all non-hydrogen[2]	0.66	0.44	0.33

[1]the RMSD computed between the atoms of all amino acids that are common to both the target and the reference in the aligned and superposed structure. The amino acids need not be identical.
[2]the RMSD computed only between identical amino acids, which are common to both the target and the reference in the aligned and superposed structure.

The present invention is also directed to a three-dimensional structure of all or a portion of AKT1. This three-dimensional structure may be used to identify binding sites, to provide mutants having desirable binding properties, and ultimately, to design, characterize, or identify ligands capable of interacting with AKT1. Ligands that interact with AKT1 may be any type of atom, compound, protein or chemical group that binds to or otherwise associates with the protein. Examples of types of ligands include natural substrates for AKT1, inhibitors of AKT1, and heavy atoms. The inhibitors of AKT1 may optionally be used as drugs to treat therapeutic indications by modifying the in vivo activity of AKT1.

In various embodiments, methods are provided for displaying a three dimensional representation of a structure of a protein comprising:

taking machine readable data comprising structure coordinates that have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1;

computing a three dimensional representation of a structure based on the structure coordinates; and

displaying the three dimensional representation.

The present invention is also directed to a method for solving a three-dimensional crystal structure of a target protein using the structure of AKT1.

In various embodiments, computational methods are provided comprising:

taking machine readable data comprising structure coordinates that have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1;

computing phases based on the structural coordinates;

computing an electron density map based on the computed phases; and

determining a three-dimensional crystal structure based on the computed electron density map.

In various embodiments, computational methods are provided comprising: taking an X-ray diffraction pattern of a crystal of the target protein; and computing a three-dimensional electron density map from the X-ray diffraction pattern by molecular replacement, wherein structure coordinates used as a molecular replacement model comprise structure coordinates that have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1.

These methods may optionally further comprise determining a three-dimensional crystal structure based upon the computed three-dimensional electron density map.

The present invention is also directed to using a crystal structure of AKT1, in particular the structure coordinates of AKT1 and the surface contour defined by them, in methods for screening, designing, or optimizing molecules or other chemical entities that interact with and preferably inhibit AKT1.

One skilled in the art will appreciate the numerous uses of the inventions described herein, particularly in the areas of drug design, screening and optimization of drug candidates, as well as in determining additional unknown crystal structures. For example, a further aspect of the present invention relates to using a three-dimensional crystal structure of all or a portion of AKT1 and/or its structure coordinates to evaluate the ability of entities to associate with AKT1. The entities may be any entity that may function as a ligand and thus may be any type of atom, compound, protein (such as antibodies) or chemical group that can bind to or otherwise associate with a protein.

In various embodiments, methods are provided for evaluating a potential of an entity to associate with a protein comprising:

creating a computer model of a protein structure using structure coordinates that comprise structure coordinates that have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1;

performing a fitting operation between the entity and the computer model; and

analyzing results of the fitting operation to quantify an association between the entity and the model.

In other embodiments, methods are provided for identifying entities that can associate with a protein comprising:

generating a three-dimensional structure of a protein using structure coordinates that comprise structure coordinates that have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1;

employing the three-dimensional structure to design or select an entity that can associate with the protein; and

contacting the entity with a protein wherein at least a portion of the protein has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with residues 29 to 370 of SEQ. ID No. 3.

In still other embodiments, methods are provided for identifying entities that can associate with a protein comprising:

generating a three-dimensional structure of a protein using structure coordinates that comprise structure coordinates that have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1;

employing the three-dimensional structure to design or select an entity that can associate with the protein; and

contacting the entity with a protein wherein at least a portion of the protein has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with residues 29 to 350 of SEQ. ID No. 5.

In other embodiments, methods are provided for identifying entities that can associate with a protein comprising:

generating a three-dimensional structure of a protein using structure coordinates that comprise structure coordinates that have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1; and

employing the three-dimensional structure to design or select an entity that can associate with the protein.

In other embodiments, methods are provided for identifying entities that can associate with a protein comprising:

computing a computer model for a protein binding pocket, at least a portion of the computer model having a surface contour that has a root mean square deviation equal to or less than a given RMSD value specified in Columns 3, 4 or 5 of Table 1 when the coordinates used to compute the surface contour are compared to the structure coordinates of FIG. **3**, wherein (a) the root mean square deviation is calculated by the calculation method set forth herein, (b) the portion of amino acid residues associated with the given RMSD value in Table 1 (specified in Column 2 of Table 1) are superimposed according to the RMSD calculation, and (c) the root mean square deviation is calculated based only on those amino acid residues present in both the protein being modeled and the portion of the protein associated with the given RMSD in Table 1 (specified in Column 1 of Table 1);

employing the computer model to design or select an entity that can associate with the protein; and

contacting the entity with a protein wherein at least a portion of the protein has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with residues 29 to 370 of SEQ. ID No. 3.

In yet other embodiments, methods are provided for identifying entities that can associate with a protein comprising:

computing a computer model for a protein binding pocket, at least a portion of the computer model having a surface contour that has a root mean square deviation equal to or less than a given RMSD value specified in Columns 3, 4 or 5 of Table 1 when the coordinates used to compute the surface contour are compared to the structure coordinates of FIG. **3**, wherein (a) the root mean square deviation is calculated by the calculation method set forth herein, (b) the portion of amino acid residues associated with the given RMSD value in Table 1 (specified in Column 2 of Table 1) are superimposed according to the RMSD calculation, and (c) the root mean square deviation is calculated based only on those amino acid residues present in both the protein being modeled and the portion of the protein associated with the given RMSD in Table 1 (specified in Column 1 of Table 1);

employing the computer model to design or select an entity that can associate with the protein; and

contacting the entity with a protein wherein at least a portion of the protein has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with residues 29 to 350 of SEQ. ID No. 5.

In other embodiments, methods are provided for identifying entities that can associate with a protein comprising:

computing a computer model for a protein binding pocket, at least a portion of the computer model having a surface contour that has a root mean square deviation equal to or less than a given RMSD value specified in Columns 3, 4 or 5 of Table 1 when the coordinates used to compute the surface contour are compared to the structure coordinates of FIG. **3**, wherein (a) the root mean square deviation is calculated by the calculation method set forth herein, (b) the portion of amino acid residues associated with the given RMSD value in Table 1 (specified in Column 2 of Table 1) are superimposed according to the RMSD calculation, and (c) the root mean square deviation is calculated based only on those amino acid residues present in both the protein being modeled and the portion of the protein associated with the given RMSD in Table 1 (specified in Column 1 of Table 1); and

employing the computer model to design or select an entity that can associate with the protein.

In other embodiments, methods are provided for evaluating the ability of an entity to associate with a protein, the methods comprising:

constructing a computer model defined by structure coordinates that have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1;

selecting an entity to be evaluated by a method selected from the group consisting of (i) assembling molecular fragments into the entity, (ii) selecting an entity from a small molecule database, (iii) de novo ligand design of the entity, and (iv) modifying a known ligand for AKT1, or a portion thereof;

performing a fitting program operation between computer models of the entity to be evaluated and the binding pocket in order to provide an energy-minimized configuration of the entity in the binding pocket; and

evaluating the results of the fitting operation to quantify the association between the entity and the binding pocket model in order to evaluate the ability of the entity to associate with the binding pocket.

In other embodiments, methods are provided for evaluating the ability of an entity to associate with a protein, the methods comprising:

computing a computer model for a protein binding pocket, at least a portion of the computer model having a surface contour that has a root mean square deviation equal to or less than a given RMSD value specified in Columns 3, 4 or 5 of Table 1 when the coordinates used to compute the surface contour are compared to the structure coordinates of FIG. **3**, wherein (a) the root mean square deviation is calculated by the calculation method set forth herein, (b) the portion of amino acid residues associated with the given RMSD value in Table 1 (specified in Column 2 of Table 1) are superimposed according to the RMSD calculation, and (c) the root mean square deviation is calculated based only on those amino acid residues present in both the protein being modeled and the portion of the protein associated with the given RMSD in Table 1 (specified in Column 1 of Table 1);

selecting an entity to be evaluated by a method selected from the group consisting of (i) assembling molecular fragments into the entity, (ii) selecting an entity from a small molecule database, (iii) de novo ligand design of the entity, and (iv) modifying a known ligand for AKT1, or a portion thereof;

performing a fitting program operation between computer models of the entity to be evaluated and the binding pocket in order to provide an energy-minimized configuration of the entity in the binding pocket; and

evaluating the results of the fitting operation to quantify the association between the entity and the binding pocket model in order to evaluate the ability of the entity to associate with the binding pocket.

In regard to each of these embodiments, the protein may optionally have activity characteristic of AKT1. For example, the protein may optionally be inhibited by inhibitors of wild type AKT1.

In another embodiment, a method is provided for identifying an entity that associates with a protein comprising: taking structure coordinates from diffraction data obtained from a crystal of a protein wherein at least a portion of the protein has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with residues 29 to 370 of SEQ. ID No. 3; and performing rational drug design using a three dimensional structure that is based on the obtained structure coordinates.

In another embodiment, a method is provided for identifying an entity that associates with a protein comprising: taking structure coordinates from diffraction data obtained from a crystal of a protein wherein at least a portion of the protein has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with residues 29 to 350 of SEQ. ID No. 5; and performing rational drug design using a three dimensional structure that is based on the obtained structure coordinates.

The protein crystals may optionally have a crystal lattice with a C2 space group and unit cell dimensions, +/−5%, of a=153.000 Å, b=79.597 Å, c=103.363 Å, α=90.00, β=123.16, γ=90.00 degrees.

The protein crystals may optionally have a crystal lattice with a P1 space group and unit cell dimensions, +/−5%, of a=44.045 Å, b=45.247 Å, c=101.445 Å, α=88.41, β=78.93, γ=72.99 degrees.

The method may optionally further comprise selecting one or more entities based on rational drug design and contacting the selected entities with the protein. The method may also optionally further comprise measuring an activity of the protein when contacted with the one or more entities. The method also may optionally further comprise comparing activity of the protein in the presence of and in the absence of the one or more entities; and selecting entities where activity of the protein changes depending upon whether a particular entity is present. The method also may optionally further comprise contacting cells expressing the protein with the one or more entities and detecting a change in a phenotype of the cells when a particular entity is present.

BRIEF DESCRIPTION OF THE FIGURES

FIG. **1** illustrates SEQ. ID Nos. 1, 2, 3, 4 and 5 referred to in this application.

FIG. **2**A illustrates crystals of AKT1 corresponding to SEQ. ID No. 3, having a crystal lattice in a C2 space group and unit cell dimensions, +/−5%, of a=153.000 Å, b=79.597 Å, c=103.363 Å, α=90.00, β=123.16, γ=90.00 degrees.

FIG. **2**B illustrates a crystal of AKT1 corresponding to SEQ. ID No. 5, having a crystal lattice in a P1 space group and unit cell dimensions, +/−5%, a=44.045 Å, b=45.247 Å, c=101.445 Å, α=88.41, β=78.93, γ=72.99 degrees.

FIG. **3** lists sets of atomic structure coordinates for AKT1 as derived by X-ray crystallography from a crystal that comprises the protein of SEQ ID NO:3 (the numbering of the amino acid residues is according to SEQ ID NO:1). The following abbreviations are used in FIG. **3**: "X, Y, Z" crystallographically define the atomic position of the element measured: "B" is a thermal factor that measures movement of the atom around its atomic center; and "Occ" is an occupancy factor that refers to the fraction of the molecules in which each atom occupies the position specified by the coordinates (a value of "1" indicates that each atom has the same conformation, i.e., the same position, in all molecules of the crystal).

FIG. **4**A illustrates a ribbon diagram overview of the structures of AKT1 from SEQ. ID No. 3, highlighting secondary structural elements of the protein.

FIG. **4**B illustrates a ribbon diagram overview of the structures of AKT1 from SEQ. ID No. 5, highlighting secondary structural elements of the protein.

FIG. **5** illustrates the nucleotide binding site of AKT1 (SEQ ID NO:1) based on the determined crystal structure for the molecule in the asymmetric unit corresponding to the coordinates shown in FIG. **3**.

FIG. **6** illustrates a system that may be used to carry out instructions for displaying a crystal structure of AKT1 SEQ ID NO:1) encoded on a storage medium.

DETAILED DESCRIPTION OF THE INVENTION

The present invention relates to a member of a family of serine/threonine protein kinases and more specifically to a particular protein kinase known as Protein Kinase Bα/AKT1 (AKT1). Provided is AKT1 in crystalline form, methods of forming crystals comprising AKT1, methods of using crystals comprising AKT1, a crystal structure of AKT1, and methods of using the crystal structure.

In describing protein structure and function herein, reference is made to amino acids comprising the protein. The amino acids may also be referred to by their conventional abbreviations; A=Ala=Alanine; T=Thr=Threonine; V=Val=Valine; C=Cys=Cysteine; L=Leu=Leucine; Y=Tyr=Tyrosine; I=Ile=Isoleucine; N=Asn=Asparagine; P=Pro=Proline; Q=Gln=Glutamine; F=Phe=Phenylalanine; D=Asp=Aspartic Acid; W=Trp=Tryptophan; E=Glu=Glutamic Acid; M=Met=Methionine; K=Lys=Lysine; G=Gly=Glycine; R=Arg=Arginine; S=Ser=Serine; and H=His=Histidine.

1. AKT1

The AKT or protein Kinase B (PKB) family of serine/threonine protein kinases is comprised of 3 highly homologous members, AKT1/PKBα, AKT2/PKBβ and AKT3/PKBγ. The family of AKT proteins are involved in signal transduction pathways that regulate cellular processes including apoptosis, proliferation, differentiation and metabolism. Expression of AKT family members have been found to be altered in many human malignant carcinomas including gastric, breast, prostate, ovarian and pancreatic. AKT1 is the cellular homolog for the viral oncogene (v-AKT) that causes leukemia in mice, whereas AKT1 is overexpressed in 20% of gastric adenocarcinomas (Staal, S. P. (1987) *Proc. Natl. Acad. Sci. U. S. A.* 84, 5034-5037). The AKT proteins are activated via the phosphatidylinositol 3-kinase (PI-3K) second messenger system. PI-3K generates polyphosphatidylinositides with a 3'-phosphate. The AKT proteins interact with 3'-phosphorylated phosphoinositides through their pleckstrin homology domains, which targets them to the cellular membrane where they become phosphorylated on two specific residues. For AKT1, these residues are Thr 308, within the P-loop of the protein kinase domain, and Ser 473, within the C-terminal hydrophobic motif. These phosphorylation events relieve the intracellular inhibition of AKT1 resulting in active kinase. Mutation of either of these residues to alanine inactivates AKT1, whereas substitution of these residues with aspartic acid results in partially active kinase independent of the PI-3K second messenger (Alessi, D. R., Andjelkovic, M., Caudwell, B., Cron, P., Morrice, N., Cohen, P. and Hemmings, B. A. (1996) EMBO J. 15, 6541-6551)

In one embodiment, AKT1 comprises a form of AKT1 comprising residues 138 to 480 containing the kinase domains and the C-terminal hydrophobic motif, set forth herein as SEQ. ID No. 3 that is derived from the wild-type full-length AKT1 protein (GenBank Accession Number NM_005163; Staal, S. P. (1987), "Molecular cloning of the akt oncogene and its human homologues Akt1 and Akt2: amplification of AKT1 in a primary human gastric adenocarcinoma *Proc. Natl. Acad. Sci. U.S.A.* 84, 5034-5037).

In another embodiment, AKT1 comprises residues 29 to 350 of SEQ. ID No. 5 which comprises the kinase domains of wild-type AKT1, with an engineered C-terminus in which the natural hydrophobic motif has been replaced with an engineered sequence (PIFtide).

It should be recognized that the invention may be readily extended to various variants of wild-type AKT1 and variants of fragments thereof. In another embodiment, AKT1 comprises a sequence wherein at least a portion of the sequence has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with SEQ. ID No. 1.

It is also noted that the above sequences of AKT1 are also intended to encompass isoforms, mutants and fusion proteins of these sequences. Example of fusion proteins are provided by SEQ. ID No. 3 and SEQ. ID No. 5, which include a 6 residue N-terminal tag (6 residues are histidine) and a rTev cleavage site that may be used to facilitate purification of the protein.

With the crystal structure provided herein, it is now known where amino acid residues are positioned in the structure. As a result, the impact of different substitutions can be more easily predicted and understood.

For example, based on the crystal structure, applicants have determined that the AKT1 amino acids shown in Table 2 encompass a 4-Angstrom radius around the AKT1 active site and thus are likely to interact with any active site inhibitor of AKT1. Applicants have also determined that the amino acids of Table 3 encompass a 7-Angstrom radius around the AKT1 active site. Further it has been determined that the amino acids of Table 4 encompass a 10-Angstrom radius around the AKT1 active site. It is noted that there is one AKT1 molecule in the asymmetric unit, referred to as chain A. Structural coordinates appear in FIG. **3**. It is noted that the sequence and structure of the residues in the active site may also be conserved and hence pertinent to other AKT1 variants and homologs.

One or more of the sets of amino acids set forth in the tables is preferably conserved in a variant of AKT1. Hence, AKT1 may optionally comprise a sequence wherein at least a portion of the sequence has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with any one of the above sequences (e.g., all of SEQ. ID No. 1; residues 29 to 370 of SEQ. ID No. 3; or residues 29 to 350 of SEQ. ID No. 5) where at least the residues shown in Tables 2, 3, and/or 4 are conserved with the exception of 0, 1, 2, 3, or 4 residues. It should be recognized that one might optionally vary some of the binding site residues in order to determine the effect such changes have on structure or activity.

TABLE 2

Amino Acids encompassed by a 4-Angstrom radius around the AKT1 active site (SEQ ID NO:1).

LEU 156	GLY 157	GLY 159
GLY 162	VAL 164	ALA 177
LYS 179	THR 211	MET 227
GLU 228	TYR 229	ALA 230
GLU 234	ASP 274	LYS 276
GLU 278	ASN 279	MET 281
THR 291	ASP 292	PHE 438

TABLE 3

Amino Acids encompassed by a 7-Angstrom radius around the AKT1 active site (SEQ ID NO:1).

LEU 156	GLY 157	GLY 159
GLY 162	VAL 164	ALA 177
LYS 179	THR 211	MET 227
GLU 228	TYR 229	ALA 230
GLU 234	ASP 274	LYS 276
GLU 278	ASN 279	MET 281
THR 291	ASP 292	PHE 438
THR 160	PHE 161	LYS 163
ILE 165	TYR 176	MET 178
LEU 181	GLU 198	ALA 212
ASN 231	GLY 232	GLY 233
TYR 272	LEU 282	LYS 289
PHE 293	GLY 294	LEU 295
THR 312	TYR 437	PHE 442
LYS 158		

TABLE 4

Amino Acids encompassed by a 10-Angstrom radius around the AKT1 active site (SEQ ID NO:1).

LEU 156	GLY 157	GLY 159
GLY 162	VAL 164	ALA 177
LYS 179	THR 211	MET 227
GLU 228	TYR 229	ALA 230
GLU 234	ASP 274	LYS 276
GLU 278	ASN 279	MET 281
THR 291	ASP 292	PHE 438
THR 160	PHE 161	LYS 163
ILE 165	TYR 176	MET 178
LEU 181	GLU 198	ALA 212
ASN 231	GLY 232	GLY 233
TYR 272	LEU 282	LYS 289
PHE 293	GLY 294	LEU 295
THR 312	TYR 437	PHE 442
LYS 154	LEU 155	LEU 166
VAL 167	TYR 175	ILE 180
VAL 185	ILE 186	GLU 191
HIS 194	THR 195	LEU 202
LEU 210	LEU 213	LYS 214
PHE 225	VAL 226	LEU 235
PHE 236	PHE 237	HIS 238
ARG 273	LEU 275	LEU 277
LEU 280	ASP 283	LYS 284
ILE 290	CYS 296	CYS 310
GLY 311	PRO 313	TYR 315
GLU 432	ASP 434	THR 435
ASP 439	THR 443	TRP 480
LYS 158		

With the benefit of the crystal structure and guidance provided by Tables 2, 3 and 4, a wide variety of AKT1 variants (e.g., insertions, deletions, substitutions, etc.) that fall within the above specified identity ranges may be designed and manufactured utilizing recombinant DNA techniques well known to those skilled in the art, particularly in view of the knowledge of the crystal structure provided herein. These modifications can be used in a number of combinations to produce the variants. The present invention is useful for crystallizing and then solving the structure of the range of variants of AKT1.

Variants of AKT1 may be insertional variants in which one or more amino acid residues are introduced into a predetermined site in the AKT1 sequence. For instance, insertional variants can be fusions of heterologous proteins or polypeptides to the amino or carboxyl terminus of the subunits.

Variants of AKT1 also may be substitutional variants in which at least one residue has been removed and a different residue inserted in its place. Non-natural amino acids (i.e., amino acids not normally found in native proteins), as well as isosteric analogs (amino acid or otherwise), may optionally be employed in substitutional variants. Examples of suitable substitutions are well known in the art, such as Glu→Asp, Asp→Glu, Ser→Cys, and Cys→Ser for example.

Another class of variants is deletional variants, which are characterized by the removal of one or more amino acid residues from the AKT1 sequence.

Other variants may be produced by chemically modifying amino acids of the native protein (e.g., diethylpyrocarbonate treatment that modifies histidine residues). Preferred are chemical modifications that are specific for certain amino acid side chains. Specificity may also be achieved by blocking other side chains with antibodies directed to the side chains to be protected. Chemical modification includes such reactions as oxidation, reduction, amidation, deamidation, or substitution with bulky groups such as polysaccharides or polyethylene glycol.

Exemplary modifications include the modification of lysinyl and amino terminal residues by reaction with succinic or other carboxylic acid anhydrides. Modification with these agents has the effect of reversing the charge of the lysinyl residues. Other suitable reagents for modifying amino-containing residues include imidoesters such as methyl picolinimidate; pyridoxal phosphate; pyridoxal chloroborohydride; trinitrobenzenesulfonic acid; O-methylisourea; 2,4-pentanedione; transaminase catalyzed reaction with glyoxylate; and N-hydroxysuccinamide esters of polyethylene glycol or other bulky substitutions.

Arginyl residues may be modified by reaction with a number of reagents, including phenylglyoxal; 2,3-butanedione; 1,2-cyclohexanedione; and ninhydrin. Modification of arginine residues requires that the reaction be performed in alkaline conditions because of the high pK_a of the guanidine functional group. Furthermore, these reagents may react with the groups of lysine as well as the arginine epsilon-amino group.

Tyrosyl residues may also be modified to introduce spectral labels into tyrosyl residues by reaction with aromatic diazonium compounds or tetranitromethane, forming 0-acetyl tyrosyl species and 3-nitro derivatives, respectively. Tyrosyl residues may also be iodinated using ^{125}I or ^{131}I to prepare labeled proteins for use in radioimmunoassays.

Carboxyl side groups (aspartyl or glutamyl) may be selectively modified by reaction with carbodiimides or they may be converted to asparaginyl and glutaminyl residues by reaction with ammonium ions. Conversely, asparaginyl and glutaminyl residues may be deamidated to the corresponding aspartyl or glutamyl residues, respectively, under mildly acidic conditions. Either form of these residues falls within the scope of this invention.

Other modifications that may be formed include the hydroxylation of proline and lysine, phosphorylation of hydroxyl groups of seryl or threonyl groups of lysine, arginine and histidine side chains (T. E. Creighton, *Proteins: Structure and Molecular Properties*, W.H. Freeman & Co., San Francisco, pp. 79-86, 1983), acetylation of the N-terminal amine and amidation of any C-terminal carboxyl group.

As can be seen, modifications of the nucleic sequence encoding AKT1 may be accomplished by a variety of well-known techniques, such as site-directed mutagenesis (see, Gillman and Smith, *Gene* 8:81-97 (1979) and Roberts, S. et al., *Nature* 328:731-734 (1987)). When modifications are made, these modifications may optionally be evaluated for their affect on a variety of different properties including, for example, solubility, crystallizability and a modification to the protein's structure and activity.

In one variation, the variant and/or fragment of wild-type AKT1 is functional in the sense that the resulting protein is capable of associating with at least one same chemical entity that is also capable of selectively associating with a protein comprising the wild-type AKT1 (e.g., residues 138 to 480 of SEQ. ID No. 1, residues 29 to 370 of SEQ. ID No. 3, or residues 29 to 350 of SEQ. ID No. 5) since this common associative ability evidences that at least a portion of the native structure has been conserved.

It is noted that the activity of the native protein need not necessarily be conserved. Rather, amino acid substitutions, additions or deletions that interfere with native activity but which do not significantly alter the three-dimensional structure of the domain are specifically contemplated by the invention. Crystals comprising such variants of AKT1, and the atomic structure coordinates obtained therefrom, can be used to identify compounds that bind to the native domain. These compounds may affect the activity of the native domain.

Amino acid substitutions, deletions and additions that do not significantly interfere with the three-dimensional structure of AKT1 will depend, in part, on the region where the substitution, addition or deletion occurs in the crystal structure. These modifications to the protein can now be made far more intelligently with the crystal structure information provided herein. In highly variable regions of the molecule, non-conservative substitutions as well as conservative substitutions may be tolerated without significantly disrupting the three-dimensional structure of the molecule. In highly conserved regions, or regions containing significant secondary structure, conservative amino acid substitutions are preferred.

Conservative amino acid substitutions are well known in the art, and include substitutions made on the basis of similarity in polarity, charge, solubility, hydrophobicity, hydrophilicity and/or the amphipathic nature of the amino acid residues involved. For example, negatively charged amino acids include aspartic acid and glutamic acid; positively charged amino acids include lysine and arginine; and amino acids with uncharged polar head groups having similar hydrophilicity values include the following: leucine; isoleucine; valine; glycine; alanine; asparagine; glutamine; serine; threonine; phenylalanine; and tyrosine. Other conservative amino acid substitutions are well known in the art.

It should be understood that the protein may be produced in whole or in part by chemical synthesis. As a result, the selection of amino acids available for substitution or addition is not limited to the genetically encoded amino acids. Indeed, mutants may optionally contain non-genetically encoded amino acids. Conservative amino acid substitutions for many of the commonly known non-genetically encoded amino acids are well known in the art. Conservative substitutions for other amino acids can be determined based on their physical properties as compared to the properties of the genetically encoded amino acids.

In some instances, it may be particularly advantageous or convenient to substitute, delete and/or add amino acid residues in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the polypeptide, etc. Such substitutions, deletions and/or additions which do not substantially alter the three dimensional structure of AKT1 will be apparent to those having skills in the art, particularly in view of the three dimensional structure of AKT1 provided herein.

2. Cloning, Expression and Purification of AKT1

The gene encoding AKT1 can be isolated from RNA, cDNA or cDNA libraries. In this case, the portion of the gene encoding amino acid residues 138 to 480 of SEQ. ID No. 1, corresponding to the kinase domains of AKT1, was isolated and is shown as SEQ. ID No. 2. In addition, the portion of the gene encoding amino acid residues 29 to 350 of SEQ. ID No. 5, corresponding to the kinase domains of an engineered AKT1, was also isolated and is shown as SEQ. ID No. 4.

Construction of expression vectors and recombinant proteins from the DNA sequence encoding AKT1 may be performed by various methods well known in the art. For example, these techniques may be performed according to Sambrook et al., Molecular Cloning-A Laboratory Manual, Cold Spring Harbor, N.Y. (1989), and Kriegler, M., Gene Transfer and Expression, A Laboratory Manual, Stockton Press, New York (1990).

A variety of expression systems and hosts may be used for the expression of AKT1. Example 1 provides one such expression system.

Once expressed, purification steps are employed to produce AKT1 in a relatively homogeneous state. In general, a higher purity solution of a protein increases the likelihood that the protein will crystallize. Typical purification methods include the use of centrifugation, partial fractionation, using salt or organic compounds, dialysis, conventional column chromatography (such as ion exchange, molecular sizing chromatography, etc.), high performance liquid chromatography (HPLC), and gel electrophoresis methods (see, e.g., Deutcher, "Guide to Protein Purification" in Methods in Enzymology (1990), Academic Press, Berkeley, Calif.).

AKT1 may optionally be affinity labeled during cloning, preferably with a N-terminal six-histidine tag and rTev cleavage site, in order to facilitate purification. With the use of an affinity label, it is possible to perform a one-step purification process on a purification column that has a unique affinity for the label. The affinity label may be optionally removed after purification. These and other purification methods are known and will be apparent to one of skill in the art.

3. Crystallization & Crystals Comprising AKT1

One aspect of the present invention relates to methods for forming crystals comprising AKT1 as well as crystals comprising AKT1.

In one embodiment, a method for forming crystals comprising AKT1 is provided comprising forming a crystallization volume comprising AKT1, one or more precipitants, optionally a buffer, optionally a monovalent and/or divalent salt and optionally an organic solvent; and storing the crystallization volume under conditions suitable for crystal formation.

In yet another embodiment, a method for forming crystals comprising AKT1 is provided comprising forming a crystallization volume comprising AKT1 in solution comprising the components shown in Table 5; and storing the crystallization volume under conditions suitable for crystal formation.

TABLE 5

Precipitant
5-50% w/v of precipitant wherein the precipitant comprises one or more members of the group consisting of PEG MME having a molecular weight range between 1000-10000, PEG having a molecular weight range between 100-10000, and 0.02-2.0 M Sodium, potassium or ammonium phosphate or sulfate.
pH
pH 4-10. Buffers that may be used include, but are not limited to tris, bicine, phosphate, cacodylate, acetate, citrate, HEPES, PIPES, MES and combinations thereof.
Additives
Optionally 0.05 to 2.5 M additives wherein the additives comprise a monovalent and/or divalent salt (for example, ammonium, potassium, sodium, lithium, magnesium, calcium, and the like)
Protein Concentration
1 mg/ml-50 mg/ml
Temperature
1° C.-25° C.

In yet another embodiment, a method for forming crystals comprising AKT1 is provided comprising forming a crystallization volume comprising AKT1; introducing crystals comprising AKT1 as nucleation sites; and storing the crystallization volume under conditions suitable for crystal formation.

Crystallization experiments may optionally be performed in volumes commonly used in the art, for example typically 15, 10, 5, 2 microliters or less. It is noted that the crystallization volume optionally has a volume of less than 1 microliter, optionally 500, 250, 150, 100, 50 or less nanoliters.

It is also noted that crystallization may be performed by any crystallization method including, but not limited to batch, dialysis and vapor diffusion (e.g., sitting drop and hanging drop) methods. Micro, macro and/or streak seeding of crystals may also be performed to facilitate crystallization.

It should be understood that forming crystals comprising AKT1 and crystals comprising AKT1 according to the invention are not intended to be limited to the wild type, full length AKT1 shown in SEQ. ID No. 1 and fragments comprising residues 29 to 370 of SEQ. ID No. 3 or residues 29 to 350 of SEQ. ID No. 5. Rather, it should be recognized that the invention may be extended to various other fragments and variants of wild-type AKT1 as described above.

It should also be understood that forming crystals comprising AKT1 and crystals comprising AKT1 according to the invention may be such that AKT1 is optionally complexed with one or more ligands and one or more copies of the same ligand. The ligand used to form the complex may be any ligand capable of binding to AKT1. In one variation, the ligand is a natural substrate. In another variation, the ligand is an inhibitor.

In one particular embodiment, AKT1 crystals have a crystal lattice in the C2 space group. AKT1 crystals may also optionally have unit cell dimensions, +/−5%, of a=153.000 Å, b=79.597 Å, c=103.363 Å, α=90.00, β=123.16, γ=90.00 degrees. AKT1 crystals also preferably are capable of diffracting X-rays for determination of atomic coordinates to a resolution of 4 Å, 3.5 Å, 3.0 Å or better.

In another embodiment, AKT1 crystals have a crystal lattice in the P1 space group. AKT1 crystals may also optionally have unit cell dimensions, +/−5%, of a=44.045 Å, b=45.247 Å, c=101.445 Å, α=88.41, β=78.93, γ=72.99 degrees. AKT1 crystals also preferably are capable of diffracting X-rays for determination of atomic coordinates to a resolution of 4 Å, 3.5 Å, 3.0 Åor better.

Crystals comprising AKT1 may be formed by a variety of different methods known in the art. For example, crystallizations may be performed by batch, dialysis, and vapor diffusion (sitting drop and hanging drop) methods. A detailed description of basic protein crystallization setups may be found in McRee, D., *Practical Protein Crystallography,* 2nd Ed. (1999), Academic Press Inc. Further descriptions regarding performing crystallization experiments are

provided in Stevens et al. (2000) *Curr. Opin. Struct. Biol.:* 10(5):558-63, and U.S. Pat. Nos. 6,296,673; 5,419,278; and 5,096,676.

In one variation, crystals comprising AKT1 are formed by mixing substantially pure AKT1 with an aqueous buffer containing a precipitant at a concentration just below a concentration necessary to precipitate the protein. One suitable precipitant for crystallizing AKT1 is polyethylene glycol (PEG), which combines some of the characteristics of the salts and other organic precipitants (see, for example, Ward et al., *J. Mol. Biol.* 98:161, 1975, and McPherson, *J. Biol. Chem.* 251:6300, 1976).

During a crystallization experiment, water is removed by diffusion or evaporation to increase the concentration of the precipitant, thus creating precipitating conditions for the protein. In one particular variation, crystals are grown by vapor diffusion in hanging drops or sitting drops. According to these methods, a protein/precipitant solution is formed and then allowed to equilibrate in a closed container with a larger aqueous reservoir having a precipitant concentration for producing crystals. The protein/precipitant solution continues to equilibrate until crystals grow.

By performing submicroliter volume sized crystallization experiments, as detailed in U.S. Pat. No. 6,296,673, effective crystallization conditions for forming crystals of a AKT1 complex were obtained. In order to accomplish this, systematic broad screen crystallization trials were performed on an AKT1 complex using the sitting drop technique. In each experiment, a 100 nL mixture of AKT1 complex and precipitant was placed on a platform positioned over a well containing 100 μL of the precipitating solution. Precipitate and crystal formation was detected in the sitting drops. Fine screening was then carried out for those crystallization conditions that appeared to produce precipitate and/or crystal in the drops.

Based on the crystallization experiments that were performed, a thorough understanding of how different crystallization conditions affect AKT1 crystallization was obtained. Based on this understanding, a series of crystallization conditions were identified that may be used to form crystals comprising AKT1. These conditions are summarized in Table 5. A particular example of crystallization conditions that may be used to form diffraction quality crystals of the AKT1 complex is detailed in Example 2. FIGS. **2**A and **2**B illustrate crystals of the AKT1 complex formed using the crystallization conditions provided in Table 5.

One skilled in the art will recognize that the crystallization conditions provided in Table 5 and Example 2 can be varied and still yield protein crystals comprising AKT1. For example, it is noted that variations on the crystallization conditions described herein can be readily determined by taking the conditions provided in Table 5 and performing fine screens around those conditions by varying the type and concentration of the components in order to determine additional suitable conditions for crystallizing AKT1, variants of AKT1, and ligand complexes thereof.

Crystals comprising AKT1 have a wide range of uses. For example, now that crystals comprising AKT1 have been produced, it is noted that crystallizations may be performed using such crystals as a nucleation site within a concentrated protein solution. According to this variation, a concentrated protein solution is prepared and crystalline material (microcrystals) is used to 'seed' the protein solution to assist nucleation for crystal growth. If the concentrations of the protein and any precipitants are optimal for crystal growth, the seed crystal will provide a nucleation site around which a larger crystal forms. Given the ability to form crystals comprising AKT1 according to the present invention, the crystals so formed can be used by this crystallization technique to initiate crystal growth of other AKT1 comprising crystals, including AKT1 complexed with other ligands.

As will be described herein in greater detail, crystals may also be used to perform X-ray or neutron diffraction analysis in order to determine the three-dimensional structure of AKT1 and, in particular, to assist in the identification of its active site. Knowledge of the binding site region allows rational design and construction of ligands including inhibitors. Crystallization and structural determination of AKT1 mutants having altered bioactivity allows the evaluation of whether such changes are caused by general structure deformation or by side chain alterations at the substitution site.

4. X-Ray Data Collection and Structure Determination

Crystals comprising AKT1 may be obtained as described above in Section 3. As described herein, these crystals may then be used to perform X-ray data collection and for structure determination.

In one embodiment, described in Example 2, crystals of AKT1 were obtained where AKT1 has the sequence of residues shown in SEQ. ID No. 3. These particular crystals were used to determine the three dimensional structure of AKT1. However, it is noted that other crystals comprising AKT1 including different AKT1 variants, fragments, and complexes thereof may also be used. In particular, crystals of AKT1 having the sequence of residues shown in SEQ. ID No. 5 were also obtained, as described below.

Diffraction data were collected from cryocooled crystals (100K) of AKT1 at the Advanced Light Source (ALS) beam line 5.0.3 using an ADSC Quantum CCD detector. The diffraction pattern of the AKT1 crystals displayed symmetry consistent with space group C2 with unit cell dimensions a=153.000 Å, b=79.597 Å, c=103.363 Å, α=90.00, β=123.16, γ=90.00 degrees (+/−5%). Data were collected and integrated to 3.15 Å with the HKL2000 program package (Otwinowski, Z. and Minor, W., *Meth. Enzymol.* 276: 307 (1997)).

In another embodiment, crystals of AKT1 were obtained where AKT1 has the sequence of residues shown in SEQ. ID No. 5. These particular crystals also were used to determine the three dimensional structure of AKT1. However, it is noted that other crystals comprising AKT1 including different AKT1 variants, fragments, and complexes thereof may also be used. In particular, crystals of AKT1 having the sequence of residues shown in SEQ. ID No. 3 were also obtained, as described above.

Diffraction data were collected from cryocooled crystals (100K) of AKT1 at the Advanced Light Source (ALS) beam line 5.0.3 using an ADSC Quantum CCD detector. The diffraction pattern of the AKT1 crystals displayed symmetry consistent with space group P**1** with unit cell dimensions=44.045 Å, b=45.247 Å, c=101.445 Å, α=88.41, β=78.93, γ=72.99 degrees (+/−5%). Data were collected and integrated to 2.25 Åwith the HKL2000 program package (Otwinowski, Z. and Minor, W., *Meth. Enzymol.* 276:307 (1997)).

The structure solution for AKT1 in the space group C**2** with unit cell dimensions a=153.000 Å, b=79.597 Å, c=103.363 Å, α=90.00, β=123.16, γ=90.00 degrees (+/−5%) was obtained by the molecular replacement method using the program AMoRE (Navaza, J. *Acta Crystallogr. A*50:157 (1994)), with the coordinates for AKT2 kinase (Yang, J., et al., *Nature: Struct. Biol.* 9:940 (2002); PDB code 1O6K) used as a search model. Using data in the resolution range 15.0 to 3.5 Å, the correct solutions were obtained yielding a correlation coefficient of 0.600 and an R-value of 0.389.

All subsequent crystallographic calculations were performed using the CCP4 program package (Collaborative Computational Project, N. The CCP4 Suite: Programs for Protein Crystallography. *Acta Crystallogr. D*50, 760-763 (1994)). The molecular replacement solutions were subjected to rigid body refinement followed by restrained least-squares refinement using the maximum likelihood method as implemented in REFMAC (Murshudov, G. N., Vagin, A. A. and Dodson E. J. *Acta Crystallogr D*53:240 (1997)). The initial refinement resulted in an R-value of 0.250 and an R_{free} value of 0.334 from which differences between the AKT1 structure and the molecular replacement model could be discerned. Multiple rounds of manual fitting of the AKT1 sequence and ordered regions not present in the initial model were performed with Xfit (McRee, D. E., *J. Struct. Biol.* 125:156 (1999)). Manual fitting was interspersed with restrained least-squares refinement in REFMAC against data from 15.0 to 3.15 Å. All stages of refinement were carried with bulk solvent corrections and anisotropic scaling, and excluded 5% of R_{free} reflections for cross-validation. The data collections and data refinement statistics are given in Table 6.

TABLE 6A

Crystal data		
Space group		C2
Unit cell dimensions		a = 153.000Å b = 79.597Å c = 103.363Å α = 90.00° β = 123.16° γ = 90.00°
Data collection		
X-ray source		ALS BL 5.0.3
Wavelength [Å]		1.00
Resolution [Å]		3.15
Observations (unique)		17948
Redundancy		3.14
Completeness	overall (outer shell)	98.6 (99.0)%
I/σ(I)	overall (outer shell)	8.5 (2.1)
R_{symm} [1]	overall (outer shell)	0.102 (.506)
Refinement		
Reflections used		16835
R-factor		20.43%
R_{free}		27.85%
r.m.s bonds		0.010Å
r.m.s angles		1.40°

During structure determination, where the unit cell dimensions were a=153.000 Å, b=79.597 Å, c=103.363 Å, α=90.00, β=123.16, γ=90.00 degrees, it was realized that the asymmetric unit comprised two AKT1 molecules. Structure coordinates were determined for this complex and the resultant set of structural coordinates from the refinement are presented in FIG. **3**. It is noted that the sequence of the structure coordinates presented in FIG. **3** differ in some regards from the sequence shown in SEQ ID No. 3. Structure coordinates are not reported for the residues 138, and 449-461 in molecule A and residues 138-140, and 447-467 in molecule B because the electron density obtained was insufficient to identify their position.

The structure solution for AKT1 in the space group P**1** with unit cell dimensions a=44.045 Å, b=45.247 Å, c=101.445 Å, α88.41, β=78.93, γ=72.99 degrees (+/−5%) was obtained by the molecular replacement method using the program AMoRE (Navaza, J. *Acta Crystallogr. A*50: 157 (1994)), with the coordinates for AKT2 kinase (Yang, J., et al., *Nature: Struct. Biol.* 9:940 (2002); PDB code 1O6K) used as a search model. Using data in the resolution range 15.0 to 3.5 Å, the correct solutions were obtained yielding a correlation coefficient of 0.435 and an R-value of 0.409. All subsequent crystallographic calculations were performed using the CCP4 program package (Collaborative Computational Project, N. The CCP4 Suite: Programs for Protein Crystallography. *Acta Crystallogr. D*50, 760-763 (1994)). The molecular replacement solutions were subjected to rigid body refinement followed by restrained least-squares refinement using the maximum likelihood method as implemented in REFMAC (Murshudov, G. N., Vagin, A. A. and Dodson E. J. *Acta Crystallogr D*53:240 (1997)). The initial refinement resulted in an R-value of 0.236 and an R_{free} value of 0.313 from which differences between the AKT1 structure and the molecular replacement model could be discerned. Multiple rounds of manual fitting of the AKT1 sequence and ordered regions not present in the initial model were performed with Xfit (McRee, D. E., *J. Struct. Biol.* 125:156 (1999)). Manual fitting was interspersed with restrained least-squares refinement in REFMAC against data from 30.0 to 2.25 Å. All stages of refinement were carried with bulk solvent corrections and anisotropic scaling, and excluded 5% of R_{free} reflections for cross-validation. The data collection and data refinement statistics are given in Table 6B.

TABLE 6B

Crystal data		
Space group		P1
Unit cell dimensions		a = 44.045Å b = 45.2477Å c = 101.445Å α = 88.41° β = 78.93° γ = 72.99°
Data collection		
X-ray source		ALS BL 5.0.3
Wavelength [Å]		1.00
Resolution [Å]		2.25
Observations (unique)		33469
Redundancy		3.68
Completeness	overall (outer shell)	95.7 (93.0)%
I/σ(I)	overall (outer shell)	15.5 (2.6)
R_{symm} [1]	overall (outer shell)	0.074 (.463)
Refinement		
Reflections used		31663
R-factor		21.69%
R_{free}		27.91%
r.m.s bonds		0.013Å
r.m.s angles		1.33°

During structure determination, where the unit cell dimensions were a=44.045 Å, b=45.247 Å, c=101.445 Å, α=88.41, β=78.93, γ=72.99 degrees, it was realized that the asymmetric unit comprised two AKT1 molecules.

Those of skill in the art understand that a set of structure coordinates (such as those in FIG. **3**) for a protein or a protein-complex or a portion thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of structure coordinates could define a similar or identical shape. Moreover, slight variations in the individual coordinates may have little effect on overall shape. In terms of binding pockets, these variations would not be expected to significantly alter the nature of ligands that could associate with those pockets. The term "binding pocket" as used herein refers to a region of the protein that, as a result of its shape, favorably associates with a ligand.

These variations in coordinates may be generated because of mathematical manipulations of the AKT1 structure coordinates. For example, the sets of structure coordinates shown in FIG. **3** could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, application of a rotation matrix, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above.

Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids or other changes in any of the components that make up the crystal could also account for variations in structure coordinates. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape should be considered to be the same. Thus, for example, a ligand that binds to the active site binding pocket of AKT1 would also be expected to bind to another binding pocket whose structure coordinates defined a shape that fell within the acceptable error.

Various computational methods may be used to determine whether a particular protein or a portion thereof (referred to here as the "target protein"), typically the binding pocket, has a high degree of three-dimensional spatial similarity to another protein (referred to here as the "reference protein") against which the target protein is being compared.

The process of comparing a target protein structure to a reference protein structure may generally be divided into three steps: 1) defining the equivalent residues and/or atoms for the target and reference proteins, 2) performing a fitting operation between the proteins; and 3) analyzing the results. These steps are described in more detail below. All structure comparisons reported herein and the structure comparisons claimed are intended to be based on the particular comparison procedure described below.

Equivalent residues or atoms can be determined based upon an alignment of primary sequences of the proteins, an alignment of their structural domains or as a combination of both. Sequence alignments generally implement the dynamic programming algorithm of Needleman and Wunsch [*J. Mol. Biol.* 48: 442-453, 1970]. For the purpose of this invention the sequence alignment was performed using the publicly available software program MOE (Chemical Computing Group Inc.) package version 2002.3. When using the MOE program, alignment was performed in the sequence editor window using the ALIGN option utilizing the following program parameters: Initial pairwise Build-up: ON, Substitution Matrix: Blosum62, Round Robin: ON, Gap Start: 7, Gap Extend: 1, Iterative Refinement: ON, Build-up: TREE-BASED, Secondary Structure: NONE, Structural Alignment: ENABLED, Gap Start: 1, Gap Extend: 0.1

Once aligned, a rigid body fitting operation is performed where the structure for the target protein is translated and rotated to obtain an optimum fit relative to the structure of the reference protein. The fitting operation uses an algorithm that computes the optimum translation and rotation to be applied to the moving structure, such that the root mean square deviation of the fit over the specified pairs of equivalent atoms is an absolute minimum. For the purpose of fitting operations made herein, the publicly available software program MOE (Chemical Computing Group Inc.) v. 2002.3 was used.

The results from this process are typically reported as an RMSD value between two sets of atoms. The term "root mean square deviation" means the square root of the arithmetic mean of the squares of deviations. It is a way to express the deviation or variation from a trend or object. As used herein, an RMSD value refers to a calculated value based on variations in the atomic coordinates of a target protein from the atomic coordinates of a reference protein or portions of thereof. The structure coordinates for AKT1, provided in FIG. **3**, are used as the reference protein in these calculations.

The same set of atoms was used for initial fitting of the structures and for computing root mean square deviation values. For example, if a root mean square deviation (RMSD) between Cα atoms of two proteins is needed, the proteins in question should be superposed only on the Cα atoms and not on any other set of atoms. Similarly, if an RMSD calculation for all atoms is required, the superposition of two structures should be performed on all atoms.

Based on a review of protein structures deposited in the Protein Databank (PDB), 1O6L was identified as having the smallest RMSD values relative to the structure coordinates described in Table 6B provided herein. Table 7 below provides a series of RMSD values that were calculated by the above described process using the structure coordinates in FIG. **3** as the reference protein and the structure coordinates from PDB code: 1O6L (Human Protein Kinase Bβ, AKT2) as the target protein.

TABLE 7

AA RESIDUES USED TO PERFORM RMSD COMPARISON WITH PDB:1VR2	PORTION OF EACH AA RESIDUE USED TO PERFORM RMSD COMPARISON WITH PDB:1O6L	RMSD [Å]
Table 2 (4 Angstrom set)	alpha-carbon atoms[1]	0.43
	main-chain atoms[1]	0.49
	all non-hydrogen[2]	0.53
Table 3 (7 Angstrom set)	alpha-carbon atoms[1]	0.50
	main-chain atoms[1]	0.57
	all non-hydrogen[2]	0.67
Table 4 (10 Angstrom set)	alpha-carbon atoms[1]	0.59
	main-chain atoms[1]	0.62
	all non-hydrogen[2]	0.79
138 to 480 of SEQ. ID No. 1	alpha-carbon atoms[1]	0.79
	main-chain atoms[1]	0.80
	all non-hydrogen[2]	1.32

[1]the RMSD computed between the atoms of all amino acids that are common to both the target and the reference in the aligned and superposed structure. The amino acids need not be identical.
[2]the RMSD computed only between identical amino acids, which are common to both the target and the reference in the aligned and superposed structure.

It is noted that mutants and variants of AKT1, as well as other protein kinases, are likely to have similar structures despite having different sequences. For example, the binding pockets of these related proteins are likely to have similar contours. Accordingly, it should be recognized that the structure coordinates and binding pocket models provided herein have utility for these other related proteins.

Accordingly, in one embodiment, the invention relates to data, computer readable media comprising data, and uses of the data where the data comprises all or a portion of the structure coordinates shown in FIG. **3** or structure coordinates having a root mean square deviation (RMSD) equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1.

As noted, there are many different ways to express the surface contours of the AKT1 structure other than by using the structure coordinates provided in FIG. **3**. Accordingly, it is noted that the present invention is also directed to any data, computer readable media comprising data, and uses of the data where the data defines a computer model for a protein binding pocket, at least a portion of the computer model having a surface contour that has a root mean square deviation equal to or less than a given RMSD value specified in Columns 3,4 or 5 of Table 1 when the coordinates used to compute the surface contour are compared to the structure coordinates of FIG. **3**, wherein (a) the root mean square deviation is calculated by the calculation method set forth herein, (b) the portion of amino acid residues associated with the given RMSD value in Table 1 (specified in Column 2 of Table 1) are superimposed according to the RMSD calculation, and (c) the root mean square deviation is calculated based only on those amino acid residues present in both the protein being modeled and the portion of the protein associated with the given RMSD in Table 1 (specified in Column 1 of Table 1).

5. AKT1 Structure

The present invention is also directed to a three-dimensional crystal structure of AKT1. This crystal structure may be used to identify binding sites, to provide mutants having desirable binding properties, and ultimately, to design, characterize, or identify ligands that interact with AKT1 as well as other structurally similar proteins.

The three-dimensional crystal structure of AKT1 may be generated, as is known in the art, from the structure coordinates shown in FIG. **3** and similar such coordinates.

During the course of structure solution, it became evident that the crystals of AKT1 of the present invention contained two AKT1 molecules in the asymmetric unit. For crystals in space group C2 comprising AKT1 corresponding to SEQ ID NO:3, the final refined coordinates include amino acid residues 139-448, 462-481 in molecule A. and residues 141-446. 468-478 in molecule B (FIG. **3**). Structure coordinates are not reported for residues 138, 449-461, in molecule A and residues 138-140, 447-467, in molecule B because the electron density obtained was insufficient to identify their position. The final coordinate set additionally includes two 10 residue GSK3β substrate peptide (SEQ ID NO:6) moieties, 38 solvent molecules modeled as water, two AMPPNP ligands, and four manganese metal ions.

FIGS. **4**A and **4**B illustrate ribbon diagram overviews of the structures of AKT1 from SEQ. ID Nos. 3 and 5, respectively, highlighting the secondary structural elements of the protein. As can be seen, the structure exhibits bilobal architecture typical of protein kinase catalytic domains. The smaller N-terminal lobe contains a five-stranded anti-parallel β-sheet (β1-β5) and a critical α-helix (αC). The C-terminal lobe contains two short β-strands (β6 and β7) and eight α-helices (αD-αK).

Kinases show considerable variability in the relative orientation of the N and C lobes, in the position and orientation of the αC helix, and in the conformation of the activation loop. This relative orientation of the N- and C-terminal lobes is important in kinase function. A catalytically active conformation is generally a closed structure in which the two lobes clamp together bringing conserved residues into catalytically optimal positions. In particular, in the active conformation, the αC helix becomes parallel with the cleft between the lobes and makes tertiary contacts with the C-lobe. In the inactive conformation, observed in several unphosphorylated kinase structures, the two lobes are spaced apart at a much higher angle and the αC helix is rotated away from the C-lobe.

For AKT1, the activation segment (also known as the activation loop) comprising residues 294-316 is fully ordered in molecules A and B in both the C2 and P1 crystal forms.

6. AKT1 Active Site and Ligand Interaction

The terms "binding site" or "binding pocket", as used herein, refer to a region of a protein that, as a result of its shape, favorably associates with a ligand or substrate. The term "AKT1-like binding pocket" refers to a portion of a molecule or molecular complex whose shape is sufficiently similar to the AKT1 binding pockets as to bind common ligands. This commonality of shape may be quantitatively defined based on a comparison to a reference point, that reference point being the structure coordinates provided herein. For example, the commonality of shape may be quantitatively defined based on a root mean square deviation (RMSD) from the structure coordinates of the backbone atoms of the amino acids that make up the binding pockets in AKT1 (as set forth in FIG. **3**).

The "active site binding pockets" or "active site" of AKT1 refers to the area on the surface of AKT1 where the substrate binds.

FIG. **5** illustrates the ATP binding site of AKT1 based on the determined crystal structure for the molecule in the asymmetric unit corresponding to the structure coordinates shown in FIG. **3**. The catalytic site for ATP is located at the interface of the two lobes (FIG. **5**).

The ATP binding site of protein kinases is a primary target for the design of small molecule inhibitors. The ATP binding site appears well conserved among protein kinases and involves residues protruding from the β1-β2-β3 sheet, helix C, the loop region linking β5 and the C-lobe, the catalytic loop, and the loop linking the C-lobe with the hydrophobic motif. The structure of the ATP binding pocket in the AKT1 complex shows considerable sequence variability with other kinases, which is reflective of diversity among kinase subfamilies. The ATP binding cleft shows subtle differences in ATP site architecture that may be explored to confer specificity of inhibition.

In resolving the crystal structure of AKT1, Applicants determined that AKT1 amino acids shown in Table 2 (above) are encompassed within a 4-Angstrom radius around the AKT1 active site and therefore are likely close enough to interact with an active site inhibitor of AKT1. Applicants have also determined that the amino acids shown in Table 3 (above) are encompassed within a 7-Angstrom radius around the AKT1 active site. Further, the amino acids shown in Table 4 (above) are encompassed within a 10-Angstrom radius around the AKT1 active site. Due to their proximity to the active site, the amino acids in the 4, 7, and/or 10 Angstrom sets are preferably conserved in variants of AKT1. While it is desirable to largely conserve these residues, it should be recognized however that variants may also involve varying 1, 2, 3, 4 or more of the residues set forth in Tables 2, 3 and 4 in order, for example, to evaluate the roles these amino acids play in the binding pocket.

With the knowledge of the AKT1 crystal structure provided herein, Applicants are able to know the contour of an AKT1 binding pocket based on the relative positioning of the 4, 7, and/or 10 Angstroms sets of amino acids. Again, it is noted that it may be desirable to form variants where 1, 2, 3, 4 or more of the residues set forth in Tables 2, 3 and 4 are varied in order to evaluate the roles these amino acids play in the binding pocket. Accordingly, any set of structure coordinates for a protein from any source shall be consid-

ered within the scope of the present invention if the structure coordinates have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1.

Accordingly, in various embodiments, the invention relates to data, computer readable media comprising data, and uses of the data where the data comprises structure coordinates that have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1.

As noted above, there are many different ways to express the surface contours of the AKT1 structure other than by using the structure coordinates provided in FIG. **3**. Accordingly, it is noted that the present invention is also directed to any data, computer readable media comprising data, and uses of the data where the data defines a computer model for a protein binding pocket, at least a portion of the computer model having a surface contour that has a root mean square deviation equal to or less than a given RMSD value specified in Columns 3, 4 or 5 of Table 1 when the coordinates used to compute the surface contour are compared to the structure coordinates of FIG. **3**, wherein (a) the root mean square deviation is calculated by the calculation method set forth herein, (b) the portion of amino acid residues associated with the given RMSD value in Table 1 (specified in Column 2 of Table 1) are superimposed according to the RMSD calculation, and (c) the root mean square deviation is calculated based only on those amino acid residues present in both the protein being modeled and the portion of the protein associated with the given RMSD in Table 1 (specified in Column 1 of Table 1).

It will be readily apparent to those of skill in the art that the numbering of amino acids in other isoforms of AKT1 may be different than that set forth for AKT1. Corresponding amino acids in other isoforms of AKT1 are easily identified by visual inspection of the amino acid sequences or by using commercially available homology software programs, as further described below.

7. System For Displaying the Three Dimensional Structure of AKT1

The present invention is also directed to machine-readable data storage media having data storage material encoded with machine-readable data that comprises structure coordinates for AKT1. The present invention is also directed to a machine readable data storage media having data storage material encoded with machine readable data, which, when read by an appropriate machine, can display a three dimensional representation of a structure of AKT1.

All or a portion of the AKT1 coordinate data shown in FIG. **3**, when used in conjunction with a computer programmed with software to translate those coordinates into the three-dimensional structure of AKT1 may be used for a variety of purposes, especially for purposes relating to drug discovery. Software for generating three-dimensional graphical representations are known and commercially available. The ready use of the coordinate data requires that it be stored in a computer-readable format. Thus, in accordance with the present invention, data capable of being displayed as the three-dimensional structure of AKT1 and/or portions thereof and/or their structurally similar variants may be stored in a machine-readable storage medium, which is capable of displaying a graphical three-dimensional representation of the structure.

For example, in various embodiments, a computer is provided for producing a three-dimensional representation of at least an AKT1-like binding pocket, the computer comprising:

machine readable data storage medium comprising a data storage material encoded with machine-readable data, the machine readable data comprising structure coordinates that have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1;

a working memory for storing instructions for processing the machine-readable data;

a central-processing unit coupled to the working memory and to the machine-readable data storage medium, for processing the machine-readable data into the three-dimensional representation; and

an output hardware coupled to the central processing unit, for receiving the three dimensional representation.

Another embodiment of this invention provides a machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when used by a machine programmed with instructions for using said data, displays a graphical three-dimensional representation comprising AKT1 or a portion or variant thereof.

In various variations, the machine readable data comprises data for representing a protein based on structure coordinates where the structure coordinates have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1.

According to another embodiment, the machine-readable data storage medium comprises a data storage material encoded with a first set of machine readable data which comprises the Fourier transform of structure coordinates that have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1, and which, when using a machine programmed

with instructions for using said data, can be combined with a second set of machine readable data comprising the X-ray diffraction pattern of another molecule or molecular complex to determine at least a portion of the structure coordinates corresponding to the second set of machine readable data. For example, the Fourier transform of the structure coordinates set forth in FIG. **3** may be used to determine at least a portion of the structure coordinates of other AKT1-like enzymes, and isoforms of AKT1.

Optionally, a computer system is provided in combination with the machine-readable data storage medium provided herein. In one embodiment, the computer system comprises a working memory for storing instructions for processing the machine-readable data; a processing unit coupled to the working memory and to the machine-readable data storage medium, for processing the machine-readable data into the three-dimensional representation; and an output hardware coupled to the processing unit, for receiving the three-dimensional representation.

FIG. **6** illustrates an example of a computer system that may be used in combination with storage media according to the present invention. As illustrated, the computer system **10** includes a computer **11** comprising a central processing unit ("CPU") **20**, a working memory **22** which may be, e.g., RAM (random-access memory) or "core" memory, mass storage memory **24** (such as one or more disk drives or CD-ROM drives), one or more cathode-ray tube ("CRT") display terminals **26**, one or more keyboards **28**, one or more input lines **30**, and one or more output lines **40**, all of which are interconnected by a conventional bi-directional system bus **50**.

Input hardware **36**, coupled to computer **11** by input lines **30**, may be implemented in a variety of ways. For example, machine-readable data of this invention may be inputted via the use of a modem or modems **32** connected by a telephone line or dedicated data line **34**. Alternatively or additionally, the input hardware **36** may comprise CD-ROM drives or disk drives **24**. In conjunction with display terminal **26**, keyboard **28** may also be used as an input device.

Conventional devices, coupled to computer **11** by output lines **40**, may similarly implement output hardware **46**. By way of example, output hardware **46** may include CRT display terminal **26** for displaying a graphical representation of a binding pocket of this invention using a program such as MOE as described herein. Output hardware might also include a printer **42**, so that hard copy output may be produced, or a disk drive **24**, to store system output for later use.

In operation, CPU **20** coordinates the use of the various input and output devices **36**, **46**; coordinates data accesses from mass storage **24** and accesses to and from working memory **22**; and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this invention. Such programs are discussed in reference to using the three dimensional structure of AKT1 described herein.

The storage medium encoded with machine-readable data according to the present invention can be any conventional data storage device known in the art. For example, the storage medium can be a conventional floppy diskette or hard disk. The storage medium can also be an optically readable data storage medium, such as a CD-ROM or a DVD-ROM, or a rewritable medium such as a magneto-optical disk that is optically readable and magneto-optically writable.

8. Uses of the Three Dimensional Structure of AKT1

The three-dimensional crystal structure of the present invention may be used to identify AKT1 binding sites, be used as a molecular replacement model to solve the structure of unknown crystallized proteins, to design mutants having desirable binding properties, and ultimately, to design, characterize, and identify entities capable of interacting with AKT1 and other structurally similar proteins as well as other uses that would be recognized by one of ordinary skill in the art. Such entities may be chemical entities or proteins. The term "chemical entity," as used herein, refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds.

The AKT1 structure coordinates provided herein are useful for screening and identifying drugs that inhibit AKT1 and other structurally similar proteins. For example, the structure encoded by the data may be computationally evaluated for its ability to associate with putative substrates or ligands. Such compounds that associate with AKT1 may inhibit AKT1, and are potential drug candidates. Additionally or alternatively, the structure encoded by the data may be displayed in a graphical three-dimensional representation on a computer screen. This allows visual inspection of the structure, as well as visual inspection of the structure's association with the compounds.

Thus, according to another embodiment of the present invention, a method is provided for evaluating the potential of an entity to associate with AKT1 or a fragment or variant thereof by using all or a portion of the structure coordinates provided in FIG. **3** or functional equivalents thereof. A method is also provided for evaluating the potential of an entity to associate with AKT1 or a fragment or variant thereof by using structure coordinates similar to all or a portion of the structure coordinates provided in FIG. **3** or functional equivalents thereof.

The method may optionally comprise the steps of: creating a computer model of all or a portion of a protein structure (e.g., a binding pocket) using structure coordinates according to the present invention; performing a fitting operation between the entity and the computer model; and analyzing the results of the fitting operation to quantify the association between the entity and the model. The portion of the protein structure used optionally comprises all of the amino acids listed in Tables 2, 3 and 4 that are present in the structure coordinates being used.

It is noted that the computer model may not necessarily directly use the structure coordinates. Rather, a computer model can be formed that defines a surface contour that is the same or similar to the surface contour defined by the structure coordinates.

The structure coordinates provided herein can also be utilized in a method for identifying a ligand (e.g., entities capable of associating with a protein) of a protein comprising an AKT1-like binding pocket. One embodiment of the method comprises: using all or a portion of the structure coordinates provided herein to generate a three-dimensional structure of an AKT1-like binding pocket; employing the three-dimensional structure to design or select a potential ligand; synthesizing the potential ligand; and contacting the synthesized potential ligand with a protein comprising an AKT1-like binding pocket to determine the ability of the potential ligand to interact with the protein. According to this method, the structure coordinates used may have a root mean square deviation equal to or less than the RMSD values specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3** according to the RMSD calculation method set forth herein, provided that

the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is calculated based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1. The portion of the protein structure used optionally comprises all of the amino acids listed in Tables 2, 3, and/or 4 that are present.

As noted previously, the three-dimensional structure of an AKT1-like binding pocket need not be generated directly from structure coordinates. Rather, a computer model can be formed that defines a surface contour that is the same or similar to the surface contour defined by the structure coordinates.

A method is also provided for evaluating the ability of an entity, such as a compound or a protein to associate with an AKT1-like binding pocket, the method comprising: constructing a computer model of a binding pocket defined by structure coordinates that have a root mean square deviation equal to or less than the RMSD value specified in Columns 3, 4 or 5 of Table 1 when compared to the structure coordinates of FIG. **3**, the root mean square deviation being calculated such that the portion of amino acid residues specified in Column 2 of Table 1 of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Column 1 of Table 1; selecting an entity to be evaluated by a method selected from the group consisting of (i) assembling molecular fragments into the entity, (ii) selecting an entity from a small molecule database, (iii) de novo ligand design of the entity, and (iv) modifying a known ligand for AKT1, or a portion thereof; performing a fitting program operation between computer models of the entity to be evaluated and the binding pocket in order to provide an energy-minimized configuration of the entity in the binding pocket; and evaluating the results of the fitting operation to quantify the association between the entity and the binding pocket model in order to evaluate the ability of the entity to associate with the binding pocket.

The computer model of a binding pocket used in this embodiment need not be generated directly from structure coordinates. Rather, a computer model can be formed that defines a surface contour that is the same or similar to the surface contour defined by the structure coordinates.

Also according to the method, the method may further include synthesizing the entity and contacting a protein having an AKT1-like binding pocket with the synthesized entity.

With the structure provided herein, the present invention for the first time permits the use of molecular design techniques to identify, select or design potential inhibitors of AKT1, based on the structure of an AKT1-like binding pocket. Such a predictive model is valuable in light of the high costs associated with the preparation and testing of the many diverse compounds that may possibly bind to the AKT1 protein.

According to this invention, a potential AKT1 inhibitor may now be evaluated for its ability to bind an AKT1-like binding pocket prior to its actual synthesis and testing. If a proposed entity is predicted to have insufficient interaction or association with the binding pocket, preparation and testing of the entity can be obviated. However, if the computer modeling indicates a strong interaction, the entity may then be obtained and tested for its ability to bind.

A potential inhibitor of an AKT1-like binding pocket may be computationally evaluated using a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the AKT1-like binding pockets.

One skilled in the art may use one of several methods to screen entities (whether chemical or protein) for their ability to associate with an AKT1-like binding pocket. This process may begin by visual inspection of, for example, an AKT1-like binding pocket on a computer screen based on the AKT1 structure coordinates in FIG. **3** or other coordinates which define a similar shape generated from the machine-readable storage medium. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within that binding pocket as defined above. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting entities. These include: GRID (P. J. Goodford, "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", J. Med. Chem., 28, pp. 849-857 (1985)) available from Oxford University, Oxford, UK; MCSS (A. Miranker et al., "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure, Function and Genetics, 11, pp. 29-34 (1991)) available from Molecular Simulations, San Diego, Calif.; AUTODOCK (D. S. Goodsell et al., "Automated Docking of Substrates to Proteins by Simulated Annealing", Proteins: Structure, Function, and Genetics, 8, pp. 195-202 (1990)) available from Scripps Research Institute, La Jolla, Calif.; and DOCK (I. D. Kuntz et al., "A Geometric Approach to Macromolecule-Ligand Interactions", J. Mol. Biol., 161, pp. 269-288 (1982)) available from University of California, San Francisco, Calif.

Once suitable entities have been selected, they can be designed or assembled. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of AKT1. This may then be followed by manual model building using software such as MOE, QUANTA or Sybyl [Tripos Associates, St. Louis, Mo].

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (P. A. Bartlett et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", in "Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196 (1989); G. Lauri and P. A. Bartlett, "CAVEAT: a Program to Facilitate the Design of Organic Molecules", J. Comput. Aided Mol. Des., 8, pp. 51-66 (1994)) available from the University of California, Berkeley, Calif.; 3D Database systems such as ISIS (MDL Information Systems, San Leandro, Calif.) reviewed in Y. C. Martin, "3D Database Searching in Drug Design", J. Med. Chem., 35, pp. 2145-2154 (1992); and HOOK (M. B. Eisen et al, "HOOK: A Program for Finding Novel Molecular Architectures that Satisfy the Chemical and Steric Requirements of a Macromolecule Binding Site", Proteins: Struct., Funct., Genet., 19, pp. 199-221 (1994)) available from Molecular Simulations, San Diego, Calif.

Instead of proceeding to build an inhibitor of an AKT1-like binding pocket in a step-wise fashion one fragment or entity at a time as described above, inhibitory or other AKT1 binding compounds may be designed as a whole or "de novo" using either an empty binding site or optionally

including some portion(s) of a known inhibitor(s). There are many de novo ligand design methods including: LUDI (H.-J. Bohm, "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. Comp. Aid. Molec. Design, 6, pp. 61-78 (1992)) available from Molecular Simulations Incorporated, San Diego, Calif.; LEGEND (Y. Nishibata et al., Tetrahedron, 47, p. 8985 (1991)) available from Molecular Simulations Incorporated, San Diego, Calif.; LEAPFROG available from Tripos Associates, St. Louis, Mo.; and SPROUT (V. Gillet et al., "SPROUT: A Program for Structure Generation)", J. Comput. Aided Mol. Design, 7, pp. 127-153 (1993)) available from the University of Leeds, UK.

Other molecular modeling techniques may also be employed in accordance with this invention (see, e.g., Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990); see also, M. A. Navia and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992); L. M. Balbes et al., "A Perspective of Modern Methods in Computer-Aided Drug Design", in Reviews in Computational Chemistry, Vol. 5, K. B. Lipkowitz and D. B. Boyd, Eds., VCH, New York, pp. 337-380 (1994); see also, W. C. Guida, "Software For Structure-Based Drug Design", Curr. Opin. Struct. Biology, 4, pp. 777-781 (1994)).

Once an entity has been designed or selected, for example, by the above methods, the efficiency with which that entity may bind to an AKT1 binding pocket may be tested and optimized by computational evaluation. For example, an effective AKT1 binding pocket inhibitor preferably demonstrates a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient AKT1 binding pocket inhibitors should preferably be designed with deformation energy of binding of not greater than about 10 kcal/mole, and more preferably, not greater than 7 kcal/mole. AKT1 binding pocket inhibitors may interact with the binding pocket in more than one of multiple conformations that are similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformations observed when the inhibitor binds to the protein.

An entity designed or selected as binding to an AKT1 binding pocket may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme and with the surrounding water molecules. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interactions. Examples of programs designed for such uses include: Gaussian 94, revision C (M. J. Frisch, Gaussian, Inc., Pittsburgh, Pa. COPYRGT.1995); AMBER, version 4.1 (P. A. Kollman, University of California at San Francisco, COPYRGT 1995); QUANTA/CHARMM (Molecular Simulations, Inc., San Diego, Calif. COPYRGT. 1995); Insight II/Discover (Molecular Simulations, Inc., San Diego, Calif. COPYRGT.1995); DelPhi (Molecular Simulations, Inc., San Diego, Calif. COPYRGT.1995); and AMSOL (Quantum Chemistry Program Exchange, Indiana University). These programs may be implemented, for instance, using a Silicon Graphics workstation such as an Indigo^2 with "IMPACT" graphics. Other hardware systems and software packages will be known to those skilled in the art.

Another approach provided by this invention, is the computational screening of small molecule databases for chemical entities or compounds that can bind in whole, or in part, to an AKT1 binding pocket. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarities or by estimated interaction energy [E. C. Meng et al., J. Comp. Chem., 13, 505-524 (1992)].

According to another embodiment, the invention provides compounds that associate with an AKT1-like binding pocket produced or identified by various methods set forth above.

The structure coordinates set forth in FIG. **3** can also be used to aid in obtaining structural information about another crystallized molecule or molecular complex. This may be achieved by any of a number of well-known techniques, including molecular replacement.

For example, a method is also provided for utilizing molecular replacement to obtain structural information about a protein whose structure is unknown comprising the steps of: generating an X-ray diffraction pattern of a crystal of the protein whose structure is unknown; generating a three-dimensional electron density map of the protein whose structure is unknown from the X-ray diffraction pattern by using at least a portion of the structure coordinates set forth in FIG. **3** as a molecular replacement model.

By using molecular replacement, all or part of the structure coordinates of the AKT1 provided by this invention (and set forth in FIG. **3**) can be used to determine the structure of another crystallized molecule or molecular complex more quickly and efficiently than attempting an ab initio structure determination. One particular use includes use with other structurally similar proteins. Molecular replacement provides an accurate estimation of the phases for an unknown structure. Phases are a factor in equations used to solve crystal structures that cannot be determined directly. Obtaining accurate values for the phases, by methods other than molecular replacement, is a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the solution of crystal structures. However, when the crystal structure of a protein containing at least a homologous portion has been solved, the phases from the known structure provide a satisfactory estimate of the phases for the unknown structure.

Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of AKT1 according to FIG. **3** within the unit cell of the crystal of the unknown molecule or molecular complex so as best to account for the observed X-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed X-ray diffraction pattern amplitudes to generate an electron density map of the structure whose coordinates are unknown. This, in turn, can be subjected to any well-known model building and structure refinement techniques to provide a final, accurate structure of the unknown crystallized molecule or molecular complex [E. Lattman, "Use of the Rotation and Translation Functions", in Meth. Enzymol., 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York (1972)].

The structure of any portion of any crystallized molecule or molecular complex that is sufficiently homologous to any portion of AKT1 can be resolved by this method.

In one embodiment, the method of molecular replacement is utilized to obtain structural information about the present

invention and any other AKT1-like molecule. The structure coordinates of AKT1, as provided by this invention, are particularly useful in solving the structure of other isoforms of AKT1 or AKT1 complexes.

The structure coordinates of AKT1 as provided by this invention are useful in solving the structure of AKT1 variants that have amino acid substitutions, additions and/or deletions (referred to collectively as "AKT1 mutants", as compared to naturally occurring AKT1). These AKT1 mutants may optionally be crystallized in co-complex with a ligand, such as an inhibitor, substrate analogue or a suicide substrate. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of AKT1. Potential sites for modification within the various binding sites of the enzyme may thus be identified. This information provides an additional tool for determining the most efficient binding interactions such as, for example, increased hydrophobic interactions, between AKT1 and a ligand. It is noted that the ligand may be the protein's natural ligand or may be a potential agonist or antagonist of a protein.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 1.5-3 Å resolution X-ray data to an R value of about 0.22 or less using computer software, such as X-PLOR [Yale University, COPYRIGHT.1992, distributed by Molecular Simulations, Inc.; see, e.g., Blundell & Johnson, supra; Meth. Enzymol., Vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985)]. This information may thus be used to optimize known AKT1 inhibitors, and more importantly, to design new AKT1 inhibitors.

The structure coordinates described above may also be used to derive the dihedral angles, phi and psi, that define the conformation of the amino acids in the protein backbone. As will be understood by those skilled in the art, the phi_n angle refers to the rotation around the bond between the alpha-carbon and the nitrogen, and the Psi_n angle refers to the rotation around the bond between the carbonyl carbon and the alpha-carbon. The subscript "n" identifies the amino acid whose conformation is being described [for a general reference, see Blundell and Johnson, Protein Crystallography, Academic Press, London, 1976].

9. Uses of the Crystal and Diffraction Pattern of AKT1

Crystals, crystallization conditions and the diffraction pattern of AKT1 that can be generated from the crystals also have a range of uses. One particular use relates to screening entities that are not known ligands of AKT1 for their ability to bind to AKT1. For example, with the availability of crystallization conditions, crystals and diffraction patterns of AKT1 provided according to the present invention, it is possible to take a crystal of AKT1; expose the crystal to one or more entities that may be a ligand of AKT1; and determine whether a ligand/AKT1 complex is formed. The crystals of AKT1 may be exposed to potential ligands by various methods, including but not limited to, soaking a crystal in a solution of one or more potential ligands or co-crystallizing AKT1 in the presence of one or more potential ligands. Given the structure coordinates provided herein, once a ligand complex is formed, the structure coordinates can be used as a model in molecular replacement in order to determine the structure of the ligand complex.

Once one or more ligands are identified, structural information from the ligand/AKT1 complex(es) may be used to design new ligands that bind tighter, bind more specifically, have better biological activity or have better safety profiles than known ligands.

In one embodiment, a method is provided for identifying a ligand that binds to AKT1 comprising: (a) attempting to crystallize a protein that comprises a sequence wherein at least a portion of the sequence has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with residues 138-480 of SEQ. ID No. 1 in the presence of one or more entities; (b) if crystals of the protein are obtained in step (a), obtaining an X-ray diffraction pattern of the protein crystal; and (c) determining whether a ligand/protein complex was formed by comparing an X-ray diffraction pattern of a crystal of the protein formed in the absence of the one or more entities to the crystal formed in the presence of the one or more entities.

In another embodiment, a method is provided for identifying a ligand that binds to AKT1 comprising: (a) attempting to crystallize a protein that comprises a sequence wherein at least a portion of the sequence has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with SEQ. ID No. 3 in the presence of one or more entities; (b) if crystals of the protein are obtained in step (a), obtaining an X-ray diffraction pattern of the protein crystal; and (c) determining whether a ligand/protein complex was formed by comparing an X-ray diffraction pattern of a crystal of the protein formed in the absence of the one or more entities to the crystal formed in the presence of the one or more entities.

In yet another embodiment, a method is provided for identifying a ligand that binds to AKT1 comprising: (a) attempting to crystallize a protein that comprises a sequence wherein at least a portion of the sequence has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with SEQ. ID No. 5 in the presence of one or more entities; (b) if crystals of the protein are obtained in step (a), obtaining an X-ray diffraction pattern of the protein crystal; and (c) determining whether a ligand/protein complex was formed by comparing an X-ray diffraction pattern of a crystal of the protein formed in the absence of the one or more entities to the crystal formed in the presence of the one or more entities.

In one embodiment, a method is provided for identifying a ligand that binds to AKT1 comprising: soaking a crystal of a protein wherein at least a portion of the protein has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with residues 138-380 of SEQ. ID No. 1 with one or more entities; determining whether a ligand/protein complex was formed by comparing an X-ray diffraction pattern of a crystal of the protein that has not been soaked with the one or more entities to the crystal that has been soaked with the one or more entities. Optionally, the method may further comprise converting the diffraction patterns into electron density maps using phases of the protein crystal and comparing the electron density maps.

In another embodiment, a method is provided for identifying a ligand that binds to AKT1 comprising: soaking a crystal of a protein wherein at least a portion of the protein has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater identity with SEQ. ID No. 3 with one or more entities; determining whether a ligand/protein complex was formed by comparing an X-ray diffraction pattern of a crystal of the protein that has not been soaked with the one or more entities to the crystal that has been soaked with the one or more entities. Optionally, the method may further comprise converting the diffraction patterns into electron density maps using phases of the protein crystal and comparing the electron density maps.

In yet another embodiment, a method is provided for identifying a ligand that binds to AKT1 comprising: soaking a crystal of a protein wherein at least a portion of the protein has 55%, 65%, 75%, 85%, 90%, 95%, 97%, 99% or greater

identity with SEQ. ID No. 5 with one or more entities; determining whether a ligand/protein complex was formed by comparing an X-ray diffraction pattern of a crystal of the protein that has not been soaked with the one or more entities to the crystal that has been soaked with the one or more entities. Optionally, the method may further comprise converting the diffraction patterns into electron density maps using phases of the protein crystal and comparing the electron density maps.

Libraries of "shape-diverse" compounds may optionally be used to allow direct identification of the ligand-receptor complex even when the ligand is exposed as part of a mixture. According to this variation, the need for time-consuming de-convolution of a hit from the mixture is avoided. More specifically, the calculated electron density function reveals the binding event, identifies the bound compound and provides a detailed 3-D structure of the ligand-receptor complex. Once a hit is found, one may optionally also screen a number of analogs or derivatives of the hit for tighter binding or better biological activity by traditional screening methods. The hit and information about the structure of the target may also be used to develop analogs or derivatives with tighter binding or better biological activity. It is noted that the ligand-AKT1 complex may optionally be exposed to additional iterations of potential ligands so that two or more hits can be linked together to make a more potent ligand. Screening for potential ligands by co-crystallization and/or soaking is further described in U.S. Pat. No. 6,297,021, which is incorporated herein by reference.

EXAMPLES

Example 1

Expression and Purification of AKT1

This example describes cloning, expression and purification of AKT1. It should be noted that a variety of other expression systems and hosts are also suitable for the expression of AKT1, as would be readily appreciated by one of skill in the art.

The portion of the gene encoding residues 138-480 of SEQ ID NO:1 (SEQ ID NO:2), which corresponds to the catalytic domain of human AKT1, was cloned into a modified pFastBacHTb vector (also known as pSXB1). In order to facilitate protein expression several site-directed mutations were introduced into the catalytic domain of human AKT1 including Met446 to Ser (M446S), and the replacement of a loop containing Glu 267-Lys 268-Asn 269 with two residues Arg267 and Asp268. In addition this construct contained a phosphomimetic Aspartic acid mutation of a hydrophobic motif serine residue (S473D). Expression from this vector produced the recombinant AKT1 catalytic domain with a 6x-histidine tag at the N-terminus followed by a rTEV protease cleavage sequence to facilitate tag removal (the excised 6x-Histidine tag and rTev cleavage site sequences are underlined in SEQ ID NO:3). Recombinant baculovirus genomic DNAs incorporating the AKT1 catalytic domain cDNA sequences were generated by transposition using the BAC-TO-BAC® Baculovirus Expression system (Invitrogen). Infectious viral particles were obtained by transfection of a 2 ml adherent culture of *Spodoptera frugiperda* Sf9 insect cells with the recombinant viral genomic DNA. Growth in ESF 921 protein free medium (Expression Systems) was for 3 days at 27° C. The resulting Passage 0 viral supernatant was used to obtain Passage 1 high titer viral stock (HTS) by infection of a 30 ml adherent culture of *Spodoptera frugiperda* Sf9 insect cells grown under similar conditions. Passage 1 HTS was used in turn to infect a 100 ml suspension culture of *Spodoptera frugiperda* Sf9 insect cells in order to generate Passage 2 HTS.

Passage 2 HTS was used to infect a 5-liter culture of *Spodoptera frugiperda* Sf9 insect cells (at a density of approx. 3×10^6 cells/ml) in a 10 liter Wave BioReactor grown in ESF-921 serum-free medium at a multiplicity of infection (moi) of approximately 5 (empirical value based on usual HTS viral counts). Cell growth/infection proceeded for two days after which time the cells were pelleted by centrifugation and the cell pellet stored at −80° C. until required. Frozen cell pellets from two such 5-liter cultures were removed from the −80° C. freezer and each suspended in 150 ml of Lysis Buffer (50 mM Tris-HCl, pH 7.9, 200 mM NaCl, 0.25 mM TCEP, 1 mM PMSF and 2 'Complete-EDTA' Roche Protease Inhibitor tablets). The suspensions were stirred for 45 min at 4° C. followed by centrifugation at 7,000 g for 1 h. To each supernatant was added 8 ml of a 50% slurry of PROBOND® (InVitrogen) nickel-chelating) resin that had been equilibrated in Lysis Buffer without protease inhibitors. The suspensions were mixed for 90 min followed by centrifugation at 640 g for 5 min. The supernatants were discarded and the resin pellets washed three times with 50 mM potassium phosphate, pH 7.9, 400 mM NaCl, 0.25 mM TCEP and 1 μg/ml leupeptin. Each resin sample was transferred to an OMN1 chromatography column (10 cm×1.5 cm diameter) at 4° C. and washed with 50 column volumes of 50 mM potassium phosphate, pH 7.9, 400 mM NaCl, 20 mM imidazole-HCl, pH 7.9, 0.25 mM TCEP and 1 μg/mL, leupeptin. The columns were subsequently washed with 5 column volumes of 50 mM Tris-HCl, pH 7.9, 400 mM NaCl, 0.25 mM TCEP and 1 μg/mL leupeptin. Target elution was effected by the addition of 50 mM Tris-HCl, pH 7.9, 400 mM NaCl, 200 mM imidazole-HCl, pH 7.9, 0.25 mM TCEP, 1 μg/mL leupeptin. The eluates were pooled and the polyhistidine purification tag removed by cleavage overnight with 100 μg/mL TEV protease during dialysis against 50 mM Tris-HCl, pH 7.9, 400 mM NaCl, 20 mM imidazole-HCl, pH 7.9, 0.25 mM TCEP and 1 μg/mL leupeptin at 4° C. The TEV-treated sample was passed by gravity flow through an 8 ml bed volume of ProBond chelating resin charged with Ni that had been equilibrated in 50 mM Tris-HCl, pH 7.9, 400 mM NaCl, 20 mM imidazole-HCl, pH 7.9, 0.25 mM TCEP and 1 μg mL leupeptin at 4° C. The unbound flow-through material was concentrated using VIVASPIN® centrifugal concentrators (ultrafiltration spin columns) (Sartorius AG). The purified protein was a mixture of unphosphorylated and monophosphorylated (~39933 (+0P) and 40013 (+1P)) species as determined by Mass Spectrograph (MS) analysis and had the correct molecular mass (~39,000) as determined by Mass Spectrograph (MS) analysis. This mixture of phosphorylated forms of AKT1 was then specifically phosphorylated on Thr-308 by treatment with a 1/50 molar ratio of PDK1 kinase in the presence of 5 mM ATP and 10 mM $MgCl_2$. Following 120 minute incubation with PDK1, AKT1 was converted into a mixture of mono and double phosphorylated proteins and the phosphorylation reaction was stopped by addition of 40 mM EDTA. The protein was dialyzed overnight against 50 mM Tris-HCl buffer, pH 7.6, 200 mM NaCl, 0.25 M TCEP. Following overnight dialysis, AKT1 was concentrated to approximately 10 mg/ml and diluted 4-fold in 50 mM Tris-HCl buffer, pH 7.6, 0.25 M TCEP to reduce the salt concentration prior to loading on an anion exchange column. The diluted sample was applied to a

PROS-HQ™ anion exchange column (Applied Biosystems) and eluted with 0-500 mM NaCl gradient over 48 fractions. Fractions containing double phosphorylated protein were pooled and diluted 10-fold with 25 mM Tris-HCl buffer, pH 7.6. 250 mM NaCl, 5 mM DTT and 0.1 mM EDTA. Following two ten-fold dilution buffer-exchanges, the purified AKT1 was concentrated to 17.9 mg/ml with a total volume of 0.120 ml (2.2 mg purified AKT1). The purified protein had the correct molecular mass (~40096+2P) as determined by Mass Spectrograph (MS) analysis, was monomeric by analytical size-exclusion chromatography (SEC) and exhibited a major band by sodium-dodecyl-sulfate polyacrylamide gel electrophoresis (SDS-PAGE) analyses.

The cDNA sequence encoding residues 29 to 350 of SEQ. ID No. 5 (SEQ. ID No. 4), which corresponds to the catalytic domain of engineered AKT1, was expressed, and the resultant protein purified, in an analogous manner to that described above for the protein produced from SEQ. ID No. 2.

Example 2

Crystallization of AKT1

This example describes the crystallization of AKT1. It is noted that the precise crystallization conditions used may be further varied, for example by performing a fine screen based on these crystallization conditions.

AKT1 protein samples (corresponding to SEQ ID NO:3) that had been treated with PDK1 kinase to phosphorylate the activation loop residue Thr 308, were incubated with 0.6 mM GSK3β substrate peptide (SEQ ID NO:6), 3 mM of the non-hydrolysable ATP analog AMPPNP and 6 mM $MnCl_2$ before setting crystallization trials. Crystals were obtained after an extensive and broad screen of conditions, followed by optimization. Diffraction quality crystals were grown in 100 nl sitting droplets using the vapor diffusion method. 50 nl comprising the AKT1-peptide-AMPPNP complex (18 mg/ml) was mixed with 50 nL from a reservoir solution (100 μl) comprising: 13% PEG 3350; 0.2M ammonium sulfate; and 0.1M HEPES buffer pH=7.5. The resulting solution was incubated over a period of two weeks at 4° C. Crystals typically appeared after 3-5 days and grew to a maximum size within 7-10 days. Single crystals were transferred, briefly, into a cryoprotecting solution containing the reservoir solution supplemented with 25% v/v ethylene glycol. Crystals were then flash frozen by immersion in liquid nitrogen and then stored under liquid nitrogen. Crystals of the AKT1 complex produced as described are illustrated in FIG. **2**A.

For AKT1 protein samples comprising SEQ.ID NO:5 that had been similarly treated with PDK1 kinase and incubated with 0.6 mM GSK3β substrate peptide (SEQ ID NO:6), 3 mM AMPPNP and 6 mM $MnCl_2$ diffraction quality crystals were grown in 100 nl sitting droplets using the vapor diffusion method. 50 nl comprising the AKT1-peptide-AMPPNP complex (13 mg/ml)) was mixed with 50 nL from a reservoir solution (100 μl) comprising: 19% PEG 3350; 0.2M potassium chloride; and 0.1M HEPES buffer pH=7.5. The resulting solution was incubated over a period of two weeks at 4° C. and single crystals transferred to a cryoprotecting solution containing the reservoir solution supplemented with 25% v/v ethylene glycol prior to flash freezing in liquid nitrogen. Crystals of the AKT1 complex produced as described are illustrated in FIG. **2**B.

While the present invention is disclosed with reference to certain embodiments and examples detailed above, it is to be understood that these embodiments and examples are intended to be illustrative rather than limiting, as it is contemplated that modifications will readily occur to skilled in the art, which modifications are intended to be within the scope of the invention and the appended claims. All patents, patent applications, papers, and books cited in this application are incorporated herein in their entirety.

SEQUENCE LISTING

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            20                  25                  30

Gly Thr Phe Ile Gly Tyr Lys Glu Arg Pro Gln Asp Val Asp Gln Arg
        35                  40                  45

Glu Ala Pro Leu Asn Asn Phe Ser Val Ala Gln Cys Gln Leu Met Lys
    50                  55                  60

Thr Glu Arg Pro Arg Pro Asn Thr Phe Ile Ile Arg Cys Leu Gln Trp
65                  70                  75                  80
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-continued

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Thr Thr Val Ile Glu Arg Thr Phe His Val Glu Thr Pro Glu Glu Arg
                85                  90                  95

Glu Glu Trp Thr Thr Ala Ile Gln Thr Val Ala Asp Gly Leu Lys Lys
            100                 105                 110

Gln Glu Glu Glu Glu Met Asp Phe Arg Ser Gly Ser Pro Ser Asp Asn
        115                 120                 125

Ser Gly Ala Glu Glu Met Glu Val Ser Leu Ala Lys Pro Lys His Arg
    130                 135                 140

Val Thr Met Asn Glu Phe Glu Tyr Leu Lys Leu Leu Gly Lys Gly Thr
145                 150                 155                 160

Phe Gly Lys Val Ile Leu Val Lys Glu Lys Ala Thr Gly Arg Tyr Tyr
                165                 170                 175

Ala Met Lys Ile Leu Lys Lys Glu Val Ile Val Ala Lys Asp Glu Val
            180                 185                 190

Ala His Thr Leu Thr Glu Asn Arg Val Leu Gln Asn Ser Arg His Pro
        195                 200                 205

Phe Leu Thr Ala Leu Lys Tyr Ser Phe Gln Thr His Asp Arg Leu Cys
    210                 215                 220

Phe Val Met Glu Tyr Ala Asn Gly Gly Glu Leu Phe Phe His Leu Ser
225                 230                 235                 240

Arg Glu Arg Val Phe Ser Glu Asp Arg Ala Arg Phe Tyr Gly Ala Glu
                245                 250                 255

Ile Val Ser Ala Leu Asp Tyr Leu His Ser Glu Lys Asn Val Val Tyr
            260                 265                 270

Arg Asp Leu Lys Leu Glu Asn Leu Met Leu Asp Lys Asp Gly His Ile
        275                 280                 285

Lys Ile Thr Asp Phe Gly Leu Cys Lys Glu Gly Ile Lys Asp Gly Ala
    290                 295                 300

Thr Met Lys Thr Phe Cys Gly Thr Pro Glu Tyr Leu Ala Pro Glu Val
305                 310                 315                 320

Leu Glu Asp Asn Asp Tyr Gly Arg Ala Val Asp Trp Trp Gly Leu Gly
                325                 330                 335

Val Val Met Tyr Glu Met Met Cys Gly Arg Leu Pro Phe Tyr Asn Gln
            340                 345                 350

Asp His Glu Lys Leu Phe Glu Leu Ile Leu Met Glu Glu Ile Arg Phe
        355                 360                 365

Pro Arg Thr Leu Gly Pro Glu Ala Lys Ser Leu Leu Ser Gly Leu Leu
    370                 375                 380

Lys Lys Asp Pro Lys Gln Arg Leu Gly Gly Gly Ser Glu Asp Ala Lys
385                 390                 395                 400

Glu Ile Met Gln His Arg Phe Phe Ala Gly Ile Val Trp Gln His Val
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Tyr Glu Lys Lys Leu Ser Pro Pro Phe Lys Pro Gln Val Thr Ser Glu
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Thr Asp Thr Arg Tyr Phe Asp Glu Glu Phe Thr Ala Gln Met Ile Thr
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cagacccacg accgcctctg ctttgtcatg gagtacgcca acgggggcga gctgttcttc 300

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cleavage site

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35 40 45

Lys Gly Thr Phe Gly Lys Val Ile Leu Val Lys Glu Lys Ala Thr Gly
50 55 60

Arg Tyr Tyr Ala Met Lys Ile Leu Lys Lys Glu Val Ile Val Ala Lys
65 70 75 80

Asp Glu Val Ala His Thr Leu Thr Glu Asn Arg Val Leu Gln Asn Ser
85 90 95

Arg His Pro Phe Leu Thr Ala Leu Lys Tyr Ser Phe Gln Thr His Asp
100 105 110

Arg Leu Cys Phe Val Met Glu Tyr Ala Asn Gly Gly Glu Leu Phe Phe
115 120 125

-continued

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His Leu Ser Arg Glu Arg Val Phe Ser Glu Asp Arg Ala Arg Phe Tyr
    130                 135                 140

Gly Ala Glu Ile Val Ser Ala Leu Asp Tyr Leu His Ser Arg Asp Val
145                 150                 155                 160

Val Tyr Arg Asp Leu Lys Leu Glu Asn Leu Met Leu Asp Lys Asp Gly
                165                 170                 175

His Ile Lys Ile Thr Asp Phe Gly Leu Cys Lys Glu Gly Ile Lys Asp
            180                 185                 190

Gly Ala Thr Met Lys Thr Phe Cys Gly Thr Pro Glu Tyr Leu Ala Pro
        195                 200                 205

Glu Val Leu Glu Asp Asn Asp Tyr Gly Arg Ala Val Asp Trp Trp Gly
    210                 215                 220

Leu Gly Val Val Met Tyr Glu Met Met Cys Gly Arg Leu Pro Phe Tyr
225                 230                 235                 240

Asn Gln Asp His Glu Lys Leu Phe Glu Leu Ile Leu Met Glu Glu Ile
                245                 250                 255

Arg Phe Pro Arg Thr Leu Gly Pro Glu Ala Lys Ser Leu Leu Ser Gly
            260                 265                 270

Leu Leu Lys Lys Asp Pro Lys Gln Arg Leu Gly Gly Gly Ser Glu Asp
        275                 280                 285

Ala Lys Glu Ile Met Gln His Arg Phe Phe Ala Gly Ile Val Trp Gln
    290                 295                 300

His Val Tyr Glu Lys Lys Leu Ser Pro Pro Phe Lys Pro Gln Val Thr
305                 310                 315                 320

Ser Glu Thr Asp Thr Arg Tyr Phe Asp Glu Glu Phe Thr Ala Gln Ser
                325                 330                 335

Ile Thr Ile Thr Pro Pro Asp Gln Asp Asp Ser Met Glu Cys Val Asp
            340                 345                 350

Ser Glu Arg Arg Pro His Phe Pro Gln Phe Asp Tyr Ser Ala Ser Ser
        355                 360                 365

Thr Ala
    370
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<210> SEQ ID NO 4
<211> LENGTH: 1014
<212> TYPE: DNA
<213> ORGANISM: Artificial
<220> FEATURE:
<223> OTHER INFORMATION: cDNA sequence encoding SEQ ID NO:5

<400> SEQUENCE: 4

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gtgatcctgg tgaaggagaa ggccacaggc cgctactacg ccatgaagat cctcaagaag    120

gaagtcatcg tggccaagga cgaggtggcc cacacactca ccgagaaccg cgtcctgcag    180

aactccaggc acccccttcct cacagccctg aagtactctt tccagaccca cgaccgcctc    240

tgctttgtca tggagtacgc caacgggggc gagctgttct tccacctgtc ccgggaacgt    300

gtgttctccg aggaccgggc ccgcttctat ggcgctgaga ttgtgtcagc cctggactac    360

ctgcactcgg agaagaacgt gatgtaccgg gacctcaagc tggagaacct catgctggac    420

aaggacgggc acattaagat cacagacttc gggctgtgca aggaggggat caaggacggt    480

gccaccatga agacctttg cggcacacct gagtacctgg cccccgaggt gctggaggac    540

aatgactacg gccgtgcagt ggactggtgg gggctgggcg tggtcatgta cgagatgatg    600
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tgcggtcgcc tgcccttcta caaccaggac catgagaagc tttttgagct catcctcatg 660

gaggagatcc gcttcccgcg cacgcttggt cccgaggcca agtccttgct ttcagggctg 720

ctcaagaagg accccaagca gaggcttggc gggggctccg aggacgccaa ggagatcatg 780

cagcatcgct tctttgccgg tatcgtgtgg cagcacgtgt acgagaagaa gctcagccca 840

cccttcaagc cccaggtcac gtcggagact gacaccaggt attttgatga ggagttcacg 900

gcccagatga tcaccatcac accacctgac caagatgaca gcatggagtg tgtggacagc 960

gagcgcgagg agcaggaaat gttcagagat tttgactaca ttgctgattg gtga 1014

<210> SEQ ID NO 5
<211> LENGTH: 365
<212> TYPE: PRT
<213> ORGANISM: Artificial
<220> FEATURE:
<223> OTHER INFORMATION: Amino acid sequence with a N-terminal 6x-histidine tag, spacer region, rTEV cleavage site, and a C-terminal PIFTIDE

<400> SEQUENCE: 5

Met Ser Tyr Tyr His His His His His His Asp Tyr Asp Ile Pro Thr
1 5 10 15

Thr Glu Asn Leu Tyr Phe Gln Gly Ala Met Gly Ser Arg Val Thr Met
20 25 30

Asn Glu Phe Glu Tyr Leu Lys Leu Leu Gly Lys Gly Thr Phe Gly Lys
35 40 45

Val Ile Leu Val Lys Glu Lys Ala Thr Gly Arg Tyr Tyr Ala Met Lys
50 55 60

Ile Leu Lys Lys Glu Val Ile Val Ala Lys Asp Glu Val Ala His Thr
65 70 75 80

Leu Thr Glu Asn Arg Val Leu Gln Asn Ser Arg His Pro Phe Leu Thr
85 90 95

Ala Leu Lys Tyr Ser Phe Gln Thr His Asp Arg Leu Cys Phe Val Met
100 105 110

Glu Tyr Ala Asn Gly Gly Glu Leu Phe Phe His Leu Ser Arg Glu Arg
115 120 125

Val Phe Ser Glu Asp Arg Ala Arg Phe Tyr Gly Ala Glu Ile Val Ser
130 135 140

Ala Leu Asp Tyr Leu His Ser Glu Lys Asn Val Val Tyr Arg Asp Leu
145 150 155 160

Lys Leu Glu Asn Leu Met Leu Asp Lys Asp Gly His Ile Lys Ile Thr
165 170 175

Asp Phe Gly Leu Cys Lys Glu Gly Ile Lys Asp Gly Ala Thr Met Lys
180 185 190

Thr Phe Cys Gly Thr Pro Glu Tyr Leu Ala Pro Glu Val Leu Glu Asp
195 200 205

Asn Asp Tyr Gly Arg Ala Val Asp Trp Trp Gly Leu Gly Val Val Met
210 215 220

Tyr Glu Met Met Cys Gly Arg Leu Pro Phe Tyr Asn Gln Asp His Glu
225 230 235 240

Lys Leu Phe Glu Leu Ile Leu Met Glu Glu Ile Arg Phe Pro Arg Thr
245 250 255

Leu Gly Pro Glu Ala Lys Ser Leu Leu Ser Gly Leu Leu Lys Lys Asp
260 265 270

Pro Lys Gln Arg Leu Gly Gly Gly Ser Glu Asp Ala Lys Glu Ile Met
275 280 285

-continued

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Gln His Arg Phe Phe Ala Gly Ile Val Trp Gln His Val Tyr Glu Lys
    290                 295                 300

Lys Leu Ser Pro Pro Phe Lys Pro Gln Val Thr Ser Glu Thr Asp Thr
305                 310                 315                 320

Arg Tyr Phe Asp Glu Glu Phe Thr Ala Gln Met Ile Thr Ile Thr Pro
                325                 330                 335

Pro Asp Gln Asp Asp Ser Met Glu Cys Val Asp Ser Glu Arg Glu Glu
            340                 345                 350

Gln Glu Met Phe Arg Asp Phe Asp Tyr Ile Ala Asp Trp
        355                 360                 365


<210> SEQ ID NO 6
<211> LENGTH: 10
<212> TYPE: PRT
<213> ORGANISM: Artificial
<220> FEATURE:
<223> OTHER INFORMATION: Synthetic

<400> SEQUENCE: 6

Gly Arg Pro Arg Thr Thr Ser Phe Ala Glu
1               5                   10
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We claim:

1. An isolated non-crystalline protein consisting of SEQ ID NO:3.

2. A non-crystalline protein consisting of SEQ ID NO:3.

3. A non-crystalline mutant protein consisting of residues 138-480 of SEQ ID NO: 1, wherein said mutant protein contains the mutation of M446S and S473D, and the substitution of residues E267-K268 N269 with K267-D268.

4. An isolated non-crystalline mutant protein consisting of residues 138-480 of SEQ ID NO: 1, wherein said mutant protein contains the mutation of M446S and S473D, and the substitution of residues E267-K268-N269 with K267-D268.

* * * * *